

## SEARCH REQUEST FORM

273007

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(STIC)

Requester's Full Name: Cecilia Jaisle Examiner: \_\_\_\_\_ Date: 9-19-08  
 Art Unit: 1624 Phone Number: 2-9931 Serial Number: 1059286  
 Location (Bldg/Room): REM5A28 (Mailbox #): 5018 Results Format Preferred (circle): PAPER DIS

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: See Bib Data Sheet  
 Inventors (please provide full names): \_\_\_\_\_

Earliest Priority Date: \_\_\_\_\_

## Search Topics

Please provide a detailed statement of the subject matter to be searched as specifically as possible. The subject matter to be searched. Include distinct species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

\*For Sequence Searches Only\* Please include all pertinent information (genetic code, divisional, or issued patent numbers) along with all appropriate serial numbers.

See claims attached. Please do structure search and inventor name(s) search. Display results to show identification of source, and R<sub>N</sub> #, compound name & structure of identified compounds. Search Compound of Formula I as amended. See previous search.

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Please call with any questions

## STAFF USE ONLY

## Type of Search

## Vendors and code where applicable

Searcher: _____	HA Sequence (S) _____	STN _____	Disig _____
Searcher Phone #: _____	AA Sequence (S) _____	Quant/Orbit _____	Latit/Lev _____
Searcher Location: _____	Searcher (S) _____	Weekend _____	W/F H/Atom _____
Date Searcher Filled Up: _____	Information _____	In-house sequence systems _____	
Date Completed: _____	Litigation _____	Chemical _____	Oligomer _____
Searcher Prep & Review Thru: _____	Patent _____	Interference _____	SPDI _____
Onfile Time: _____	Other _____	Other (specify) _____	Source/Lev 6th _____
			Broader/Tradit _____

## STRUCTURE SEARCH

=> fil reg; d stat que l5; fil zcapl; d que nos l6; d ibib abs hitstr l6 1-11; fil  
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STRUCTURE FILE UPDATES: 21 SEP 2008 HIGHEST RN 1051326-19-2  
 DICTIONARY FILE UPDATES: 21 SEP 2008 HIGHEST RN 1051326-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

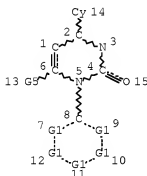
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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<http://www.cas.org/support/stngen/stndoc/properties.html>

L1 STR



VAR G1=C/N  
 VAR G5=C/NH2  
 NODE ATTRIBUTES:  
 CONNECT IS E3 RC AT 1  
 CONNECT IS E3 RC AT 3  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS UNS AT 14  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L5 397 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 94555 ITERATIONS

397 ANSWERS

SEARCH TIME: 00.00.04

FILE 'ZCAPLUS' ENTERED AT 12:36:45 ON 22 SEP 2008

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FILE COVERS 1907 - 22 Sep 2008 VOL 149 ISS 13

FILE LAST UPDATED: 21 Sep 2008 (20080921/ED)

ZCapius now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

L1 STR

L5 397 SEA FILE=REGISTRY SSS FUL L1

L6 11 SEA FILE=ZCAPLUS ABB=ON L5

L6 ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:6179 ZCAPLUS Full-text

DOCUMENT NUMBER: 148:121717

TITLE: Preparation of 1,4-diaryldihydropyrimidin-2-ones for treatment of pulmonary arterial hypertension.

INVENTOR(S): von Nussbaum, Franz; Gielen-Haertwig, Heike; Klein, Martina; Li, Volkhart; Meibom, Daniel; Sandner, Peter; Lustig, Klemens; Schaefer, Stefan

PATENT ASSIGNEE(S): Bayer Healthcare Aktiengesellschaft, Germany

SOURCE: Ger. Offen., 34pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102006031314	A1	20080103	DE 2006-102006031314	20060701
WO 2008003412	A1	20080110	WO 2007-EP5579	20070625
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

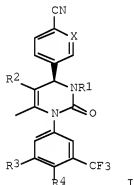
PRIORITY APPLN. INFO.:

DE 2006-102006031314A 20060701

OTHER SOURCE(S):

MARPAT 148:121717

GI



AB Use of title compds. [I; X = CH, N; R1 = (CH<sub>2</sub>)<sub>n</sub>CO<sub>2</sub>R1 3-CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>R1a, 4-CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>R1a; n = 1, 2; R1a = H, alkyl; R2 = cyano, COR<sub>2</sub>a, CO<sub>2</sub>R<sub>2</sub>a; R<sub>2</sub>a = (substituted) alkyl, cycloalkyl; R3 = H, R4 = H, F, Cl; or R3 = F, Cl and R4 = H] for use in preparation of a drug for treatment of pulmonary arterial hypertension is claimed. Thus, 5-methylhexane-2,4-dione, 4-formylbenzonitrile, and 1-[3-(trifluoromethyl)phenyl]urea were heated with polyphosphoric acid in THF overnight at 80° to give a residue which was subjected to chiral chromatog. to give 8% 4-[(4R)-5-isobutyryl-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydropyrimidin-4-yl]benzonitrile. I inhibited human neutrophil elastase with IC<sub>50</sub> = 0.9-20 nM.

IT 904958-43-6P 956487-26-8P 1000588-67-9P  
1000588-70-4P 1000588-73-7P 1000588-74-8P

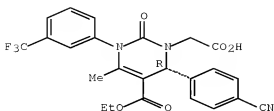
RL: SPN (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryldihydropyrimidinones for treatment of pulmonary arterial hypertension)

RN 904958-43-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

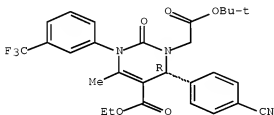
Absolute stereochemistry.



RN 956487-28-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

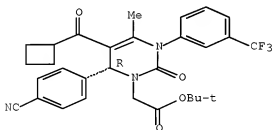
Absolute stereochemistry.



RN 1000588-67-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

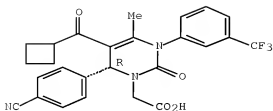
Absolute stereochemistry.



RN 1000588-70-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

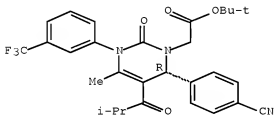
Absolute stereochemistry.



RN 1000588-73-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

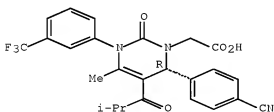
Absolute stereochemistry.



RN 1000588-74-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



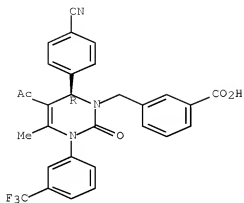
IT 864150-67-4 864150-68-5 864250-45-3

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation of diaryldihydropyrimidinones for treatment of pulmonary arterial hypertension)

RN 864150-67-4 ZCAPLUS

CN Benzoic acid, 3-[[6R]-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

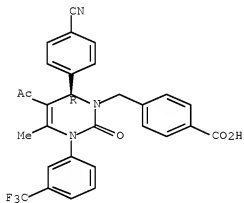
Absolute stereochemistry.



RN 864150-68-5 ZCAPLUS

CN Benzoic acid, 4-[[1(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

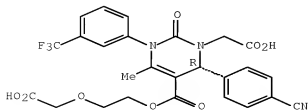
Absolute stereochemistry.



RN 864250-45-3 ZCAPLUS

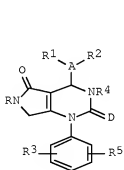
CN 1(2H)-Pyrimidineacetic acid, 5-[[2-(carboxymethoxy)ethoxy]carbonyl]-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.

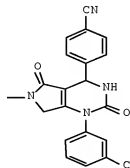


L6 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:1300977 ZCAPLUS Full-text  
 DOCUMENT NUMBER: 147:522270  
 TITLE: Preparation of tetrahydropyrrlopyrimidinediones as human neutrophil elastase (HNE) inhibitors  
 INVENTOR(S): Ray, Nicholas Charles; Finch, Harry; Edwards, Christine; O'Connor, Elizabeth  
 PATENT ASSIGNEE(S): Argenta Discovery Limited, UK  
 SOURCE: PCT Int. Appl., 73pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007129060	A1	20071115	WO 2007-GB1638	20070503
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPLN. INFO.:			GB 2006-8844	A 20060504
			GB 2006-12544	A 20060623
OTHER SOURCE(S):			MARPAT 147:522270	
GI				



I



II

AB Title compds. [I; A = aryl, heteroaryl; D = O, S; R1-R3 = H, OH, halo, NO2, cyano, alkenyl, alkynyl, alkenyloxy, (substituted) alkyl, alkoxy; R, R4 = Xm(A1)pQn(A2)q(X1)kZ; A1, A2 = (substituted) alkylene, alkenylene optionally containing O, S, NRa; Q = O, S, SO, SO2, NRa, NRaSO2, CO2, etc.; X = CO, SO2, CO2, CONRa, SO2NRa; Ra = H, alkyl, cycloalkyl; X1 = O, S, NH; Z = H,



(substituted) carbocyclyl, heterocyclyl; k, m, n, p, q = 0, 1], were prepared. Thus, title compound (II) was prepared in 3 steps from 3,5-difluorophenylurea, 4-cyanobenzaldehyde, Et acetoacetate, and methylamine. Most I inhibited HNE in the range of 1-50 nM.

IT 956487-15-3P 956487-16-4P 956487-17-5P  
956487-18-6P 956487-19-7P 956487-20-0P  
956487-21-1P 956487-22-2P 956487-23-3P  
956487-28-3P 956487-29-9P 956487-33-0P  
956487-39-1P 956487-40-4P

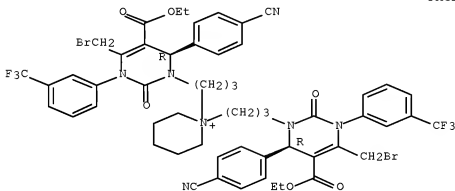
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of tetrahydropyrrolopyrimidinediones as human neutrophil elastase inhibitors)

RN 956487-15-3 ZCAPLUS

CN Piperidinium, 1,1-bis[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

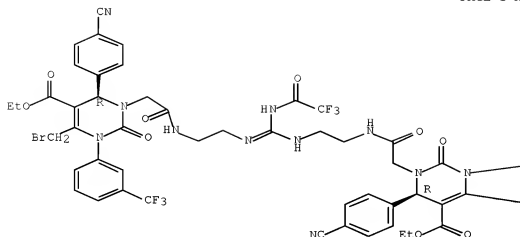


RN 956487-16-4 ZCAPLUS

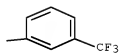
CN 5-Pyrimidinecarboxylic acid, 1,1'-[2,12-dioxo-7-[(2,2,2-trifluoroacetyl)amino]-3,6,8,11-tetraazatridec-6-ene-1,13-diyl]bis[4-(bromomethyl)-6-(4-cyanophenyl)-1,2,3,6-tetrahydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5,5'-diethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



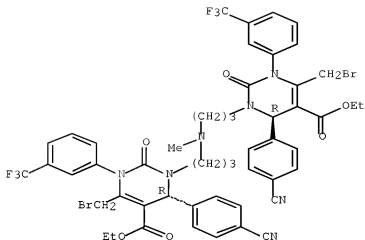
PAGE 1-B

-CH<sub>2</sub>Br

RN 956487-17-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)di-3,1-propanediyl]bis[4-(bromomethyl)-6-(4-cyanophenyl)-1,2,3,6-tetrahydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5,5'-diethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

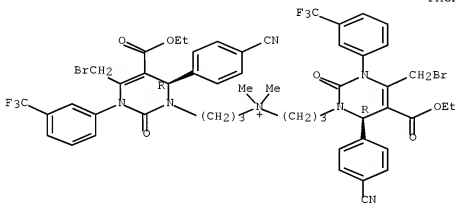


RN 956487-18-6 ZCAPLUS

CN 1(2H)-Pyrimidinepropanaminium, 4-(bromomethyl)-N-[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-N,N-dimethyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, iodide (1:1), (6R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

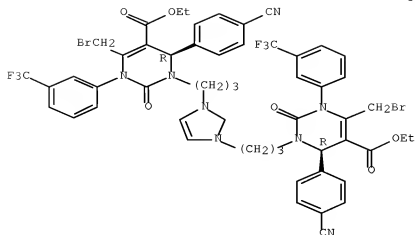
● I<sup>-</sup>

RN 956487-19-7 ZCAPLUS

CN 1H-Imidazolium, 1,3-bis[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



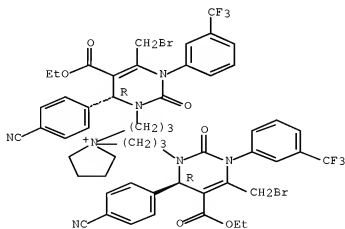
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 956487-20-0 ZCAPLUS

CN Pyrrolidinium, 1,1-bis[3-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

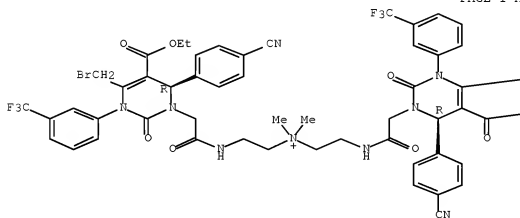


RN 956487-21-1 ZCAPLUS

CN Ethanaminium, 2-[[2-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

—CH<sub>2</sub>Br

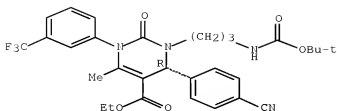
—OEt



RN 956487-22-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[3-[[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

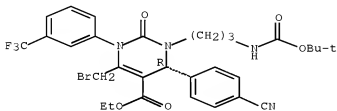
Absolute stereochemistry.



RN 956487-23-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(bromomethyl)-4-(4-cyanophenyl)-3-[3-[[[1,1-dimethylethoxy]carbonyl]amino]propyl]-1,2,3,4-tetrahydro-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

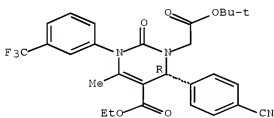
Absolute stereochemistry.



RN 956487-28-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

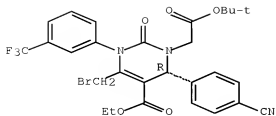
Absolute stereochemistry.



RN 956487-29-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 4-(bromomethyl)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

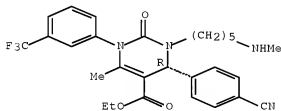
Absolute stereochemistry.



RN 956487-38-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[5-(methylamino)pentyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

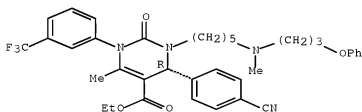
Absolute stereochemistry.



RN 956487-39-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[5-[methyl(3-phenoxypropyl)amino]pentyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

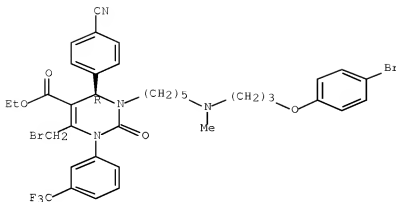
Absolute stereochemistry.



RN 956487-40-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 6-(bromomethyl)-3-[5-[[3-(4-bromophenoxy)propyl]methylamino]pentyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:1356757 ZCAPLUS Full-text  
 DOCUMENT NUMBER: 146:100714  
 TITLE: Preparation of dihydropyrimidinone multimers as human neutrophil elastase inhibitors  
 INVENTOR(S): Finch, Harry; Edwards, Christine; Ray, Nicholas Charles; Fitzgerald, Mary Frances  
 PATENT ASSIGNEE(S): Argenta Discovery Ltd., UK  
 SOURCE: PCT Int. Appl., 59pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006136857	A1	20061228	WO 2006-GB2337	20060626
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
EP 1893584	A1	20080305	EP 2006-755623	20060626
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR			
IN 2007DN10018	A	20080711	IN 2007-DN10018	20071224
CN 101243055	A	20080813	CN 2006-80030331	20080220
PRIORITY APPLN. INFO.:			GB 2005-12940	A 20050624
			WO 2006-GB2337	W 20060626

OTHER SOURCE(S): MARPAT 146:100714  
 GI



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. represented by the formula M-L-M, wherein L is a linker and each M is independently a group of formula I [A = (hetero)aryl; D = O or S; R1-R3 = independently H, halo, nitro, etc.; R4 = OH, alkyl(carbonyl), amino, etc.; Y1-Y5 = independently C or N, with the proviso that the ring in which they are comprised contains no more than 2 N atoms; R5 = (un)substituted alkyl, -O-alkyl-O-alkyl or amino; R6 = halo, nitro, cyano, etc.; and pharmaceutically acceptable salts, solvates or N-oxides thereof], were prepared as human neutrophil elastase (HNE) inhibitors. For example, II was provided in a multi-step synthesis starting from the reaction of 3-(trifluoromethyl)phenylurea with 4-cyanobenzaldehyde. I were tested for inhibitory activity towards HNE with IC50 values of 1-1000 nM. Thus, I and their pharmaceutical compns. are useful as human neutrophil elastase inhibitors for the treatment of respiratory diseases (no data).

IT 917813-97-9P 917813-99-1P 917814-01-8P

917814-02-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

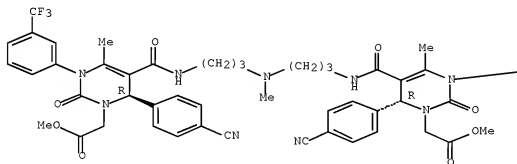
(preparation of dihydropyrimidone multimers as human neutrophil elastase inhibitors)

RN 917813-97-9 ZCAPLUS

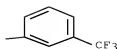
CN 1(2H)-Pyrimidineacetic acid, 5,5'-[(methylimino)bis(3,1-propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1'-dimethyl ester, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

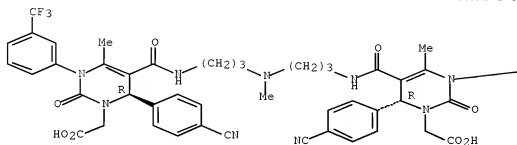


RN 917813-99-1 ZCAPLUS

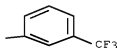
CN 1(2H)-Pyrimidineacetic acid, 5,5'-[(methylimino)bis(3,1-propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

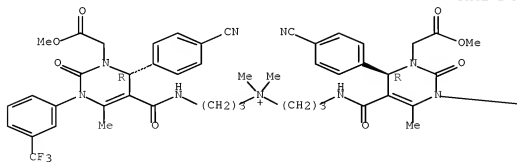


RN 917814-01-8 ZCAPLUS

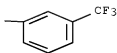
CN 1-Propanaminium, 3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(2-methoxy-2-oxoethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[[[(4R)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(2-methoxy-2-oxoethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



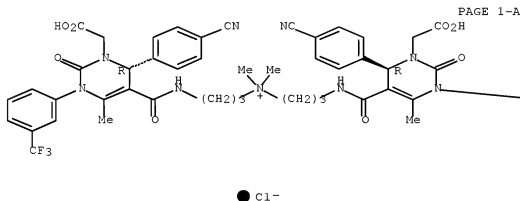
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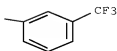
RN 917814-02-9 ZCAPLUS

CN 1-Propanaminium, 3-[[[(4R)-3-(carboxymethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]-N-[3-[[[(4R)-3-(carboxymethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, chloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-B



IT 917814-00-7P 917814-03-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

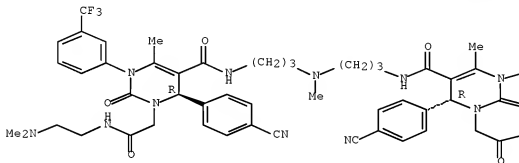
(preparation of dihydropyrimidone multimers as human neutrophil elastase  
inhibitors)

RN 917814-00-7 ZCAPLUS

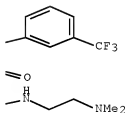
CN 1-(2H)-Pyrimidineacetamide, 5,5'-[(methylimino)bis(3,1-  
propanediyliminocarbonyl)]bis[6-(4-cyanophenyl)-N-[2-(dimethylamino)ethyl]-  
3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (CA  
INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



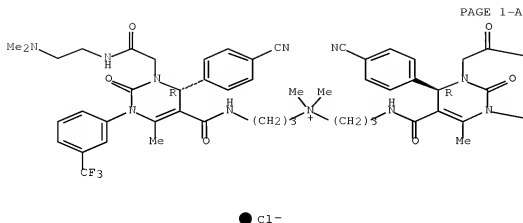
PAGE 1-B



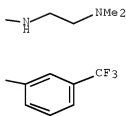
RN 917814-03-0 ZCAPLUS

CN 1-Propanaminium, 3-[[[(4R)-4-(4-cyanophenyl)-3-[2-[[2-(  
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(4-cyanophenyl)-3-[2-[[2-(dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-  
tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-  
pyrimidinyl]carbonyl]amino]propyl]-N,N-dimethyl-, chloride (1:1) (CA  
INDEX NAME)

Absolute stereochemistry.

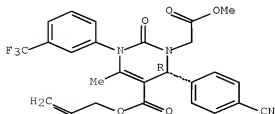


PAGE 1-B



IT 917814-23-4P 917814-24-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of dihydropyrimidone multimers as human neutrophil elastase  
 inhibitors)  
 RN 917814-23-4 ZCAPLUS  
 CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-  
 5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, methyl  
 ester, (6R)- (CA INDEX NAME)

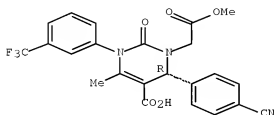
Absolute stereochemistry.



RN 917814-24-5 ZCAPLUS  
 CN 1(2H)-Pyrimidineacetic acid, 5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-

methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1-methyl ester, (6R)- (CA  
INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

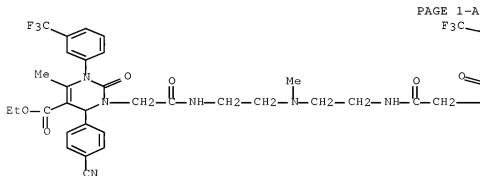
L6 ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2006:796025 ZCAPLUS [Full-text](#)  
DOCUMENT NUMBER: 145:211067  
TITLE: Multimers of tetrahydropyrimidinone compounds as  
elastase inhibitors and their preparation,  
pharmaceutical compositions, and use for treatment of  
respiratory diseases  
INVENTOR(S): Finch, Harry; Edwards, Christine; Ray, Nicholas  
Charles; O'Connor, Elizabeth Anne; Fitzgerald, Mary F.  
PATENT ASSIGNEE(S): Argenta Discovery Ltd, UK  
SOURCE: PCT Int. Appl., 132 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006082412	A2	20060810	WO 2006-GB361	20060203
WO 2006082412	A3	20061012		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
AU 2006210730	A1	20060810	AU 2006-210730	20060203
CA 2595801	A1	20060810	CA 2006-2595801	20060203
EP 1856059	A2	20071121	EP 2006-709612	20060203
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR			
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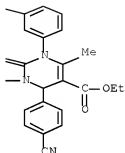
CN 101151252 A 20080326 CN 2006-80009856 20070926  
 PRIORITY APPLN. INFO.: GB 2005-2258 A 20050203  
 WO 2006-GB361 W 20060203  
 OTHER SOURCE(S): MARPAT 145:211067  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

- AB A compound of formula I is useful in therapy, e.g. of respiratory diseases. Comps. of formula I wherein L is a linker; each A are independently (un)substituted (hetero)aryl; D is O or S; each Y1 - Y5 are independently CH, CR3, CR6 or N, with the proviso that one of them is CR3, one CR6 and not more than two N per ring; each R3 are independently H, halo, NO2, CN, (un)substituted C1-6 alkyl, OH, or (un)substituted C1-6 alkoxy; each R4 are independently COCF3, (un)substituted C1-6 alkylcarbonyl, (un)substituted C1-6 alkoxycarbonyl, (un)substituted C1-6 alkenyloxy carbonyl, hydroxycarbonyl, CONH2 and derivs., (un)substituted (hetero)aryl, etc.; each R5 are independently (un)substituted C1-4 alkyl or amino; each R6 are independently halo, NO2, CN, (un)substituted C1-6 alkyl, OH, or (un)substituted C1-6 alkoxy; and their pharmaceutically acceptable salts, solvates or N-oxides thereof are claimed. Example compound II was prepared by N-alkylation of compound III with 1,12-dibromododecane. The invention compds. were evaluated for their elastase inhibitory activity. The tested compds. were shown to have desirable HNE inhibitory activity (no data).
- IT 904957-71-7P 904957-72-8P 904957-86-4P  
 904958-07-2P 904958-35-6P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (drug candidate and intermediate; preparation of multimers of tetrahydropyrimidinone compds. as elastase inhibitors useful in the treatment of respiratory diseases)
- RN 904957-71-7 ZCAPLUS
- CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



PAGE 1-B

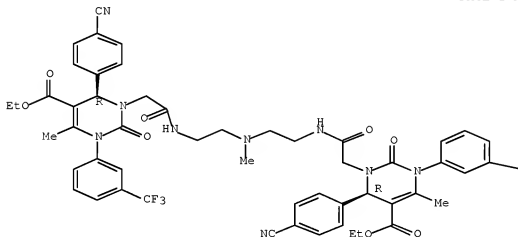


RN 904957-72-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





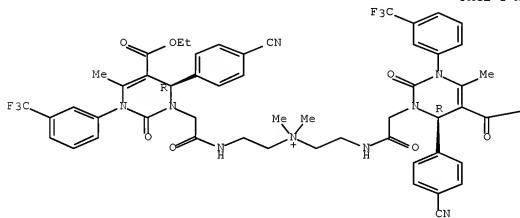
PAGE 1-B

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RN 904957-86-4 ZCAPLUS  
 CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

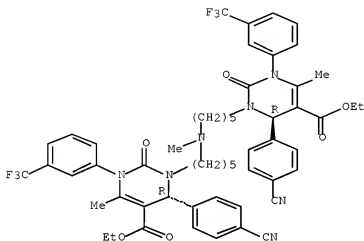
—OEt

● I<sup>-</sup>

RN 904958-07-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)di-5,1-pentanediy]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

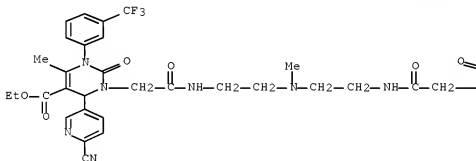
Absolute stereochemistry.

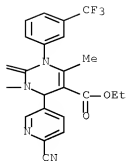


RN 904958-35-6 ZCAPLUS

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PAGE 1-A





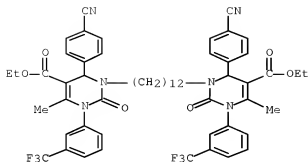
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 904958-39-0P 904958-41-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(drug candidate; preparation of multimers of tetrahydropyrimidinone compds.  
 as elastase inhibitors useful in the treatment of respiratory diseases)

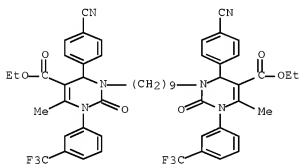
RN 904957-62-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-  
 1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl  
 ester (9CI) (CA INDEX NAME)



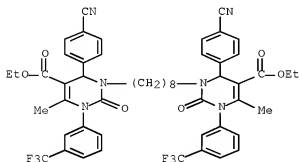
RN 904957-63-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,9-nonanediy)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



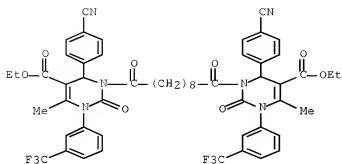
RN 904957-64-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,8-octanediy)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



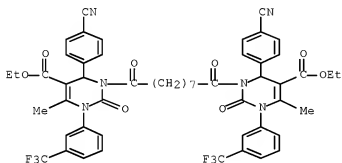
RN 904957-65-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,10-dioxo-1,10-decanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



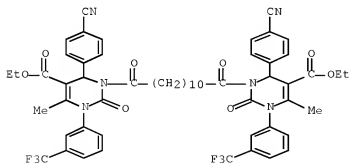
RN 904957-66-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,9-dioxo-1,9-nonanediyloxy)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904957-67-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dioxo-1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

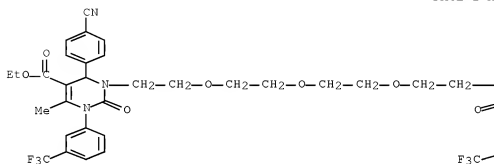


RN 904957-68-2 ZCAPLUS

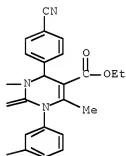
CN 5-Pyrimidinecarboxylic acid, 1,1'-(oxybis(2,1-ethanedioxy)-2,1-ethanedioxy)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

ethanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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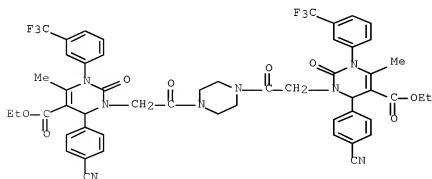


PAGE 1-B



RN 904957-69-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

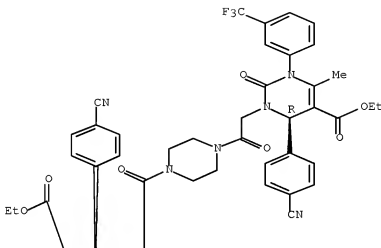


RN 904957-70-6 ZCAPLUS

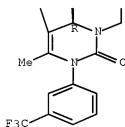
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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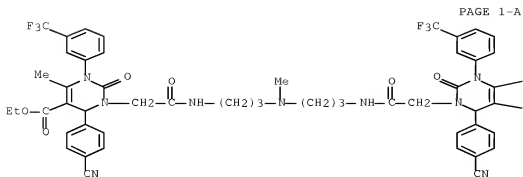


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RN 904957-73-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[3-[[3-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]propyl]methylanilino]propyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

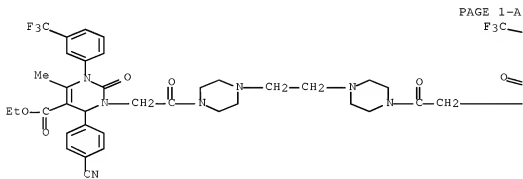


PAGE 1-B



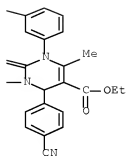
RN 904957-74-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)





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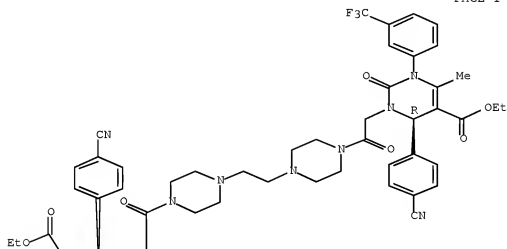


RN 904957-75-1 ZCAPLUS

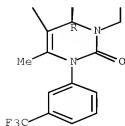
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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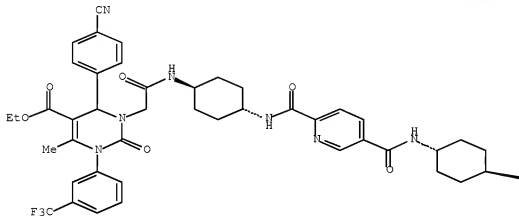


RN 904957-76-2 ZCAPLUS

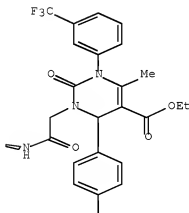
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[[trans-4-[[[5-[[[trans-4-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]cyclohexyl]amino]carbonyl]-2-pyridinyl]carbonyl]amino]cyclohexyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

Relative stereochemistry.

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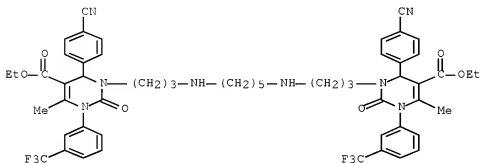


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1  
CN

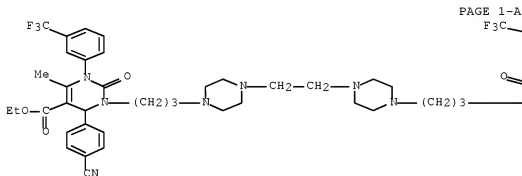
RN 904957-77-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,5-pentanediy]bis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)



RN 904957-78-4 ZCAPLUS

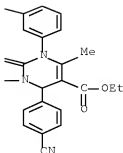
CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediyl]bis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



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F3C

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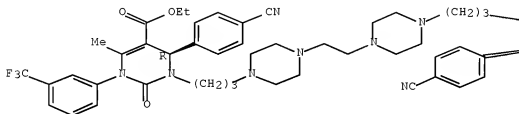


RN 904957-79-5 ZCAPLUS

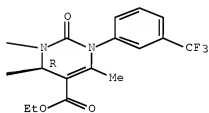
CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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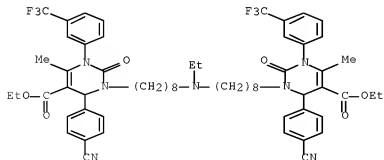


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RN 904957-80-8 ZCAPLUS

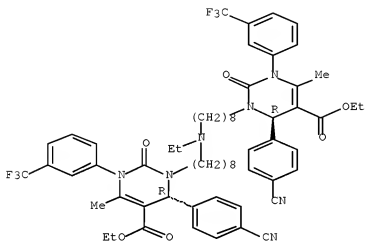
CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904957-81-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



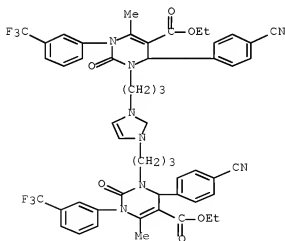
RN 904957-83-1 ZCAPLUS

CN 1H-Imidazolium, 1,3-bis[3-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 904957-82-0

CMF C53 H49 F6 N8 O6



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

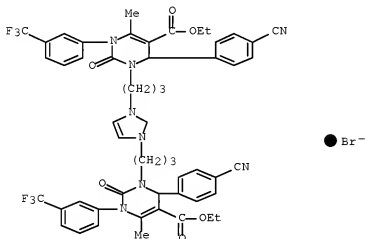
CRN 14477-72-6

CMF C2 F3 O2



RN 904957-84-2 ZCAPLUS

CN 1H-Imidazolium, 1,3-bis[3-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)



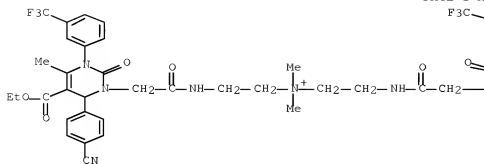
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 904957-85-3 ZCAPLUS

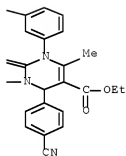
CN Ethanaminium, 2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

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F3C

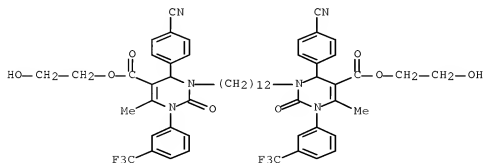


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RN 904957-87-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

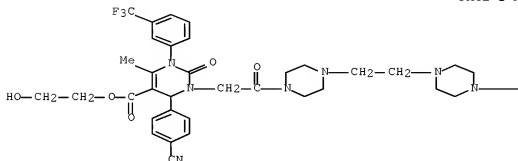


RN 904957-88-6 ZCAPLUS

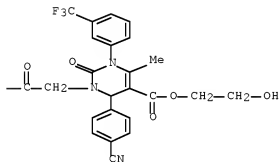
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[2-[4-[2-[6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-

(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]ethyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

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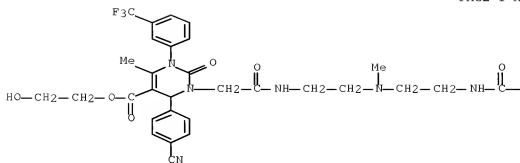


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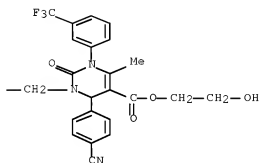
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)



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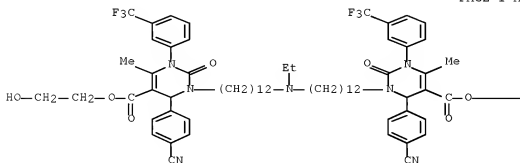
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RN 904957-90-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-12,1-dodecanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

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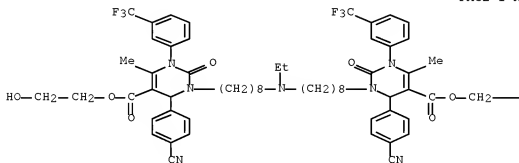


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$$-\text{CH}_2-\text{CH}_2-\text{OH}$$

RN 904957-91-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediy]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)



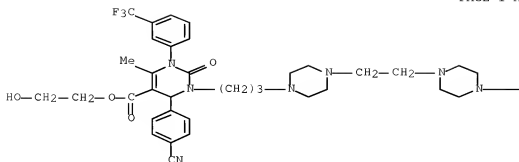
PAGE 1-B

$$\text{—CH}_2\text{—OH}$$

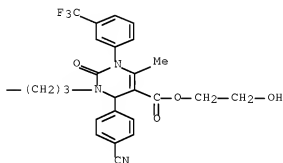
RN 904957-92-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis(2-hydroxyethyl) ester (9CI) (CA INDEX NAME)

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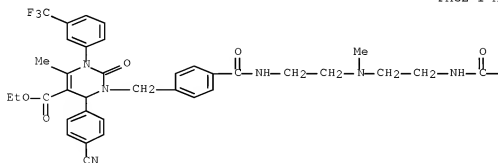
PAGE 1-B



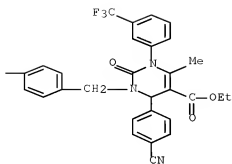
RN 904957-93-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[4-[[[2-[[2-[[4-[[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]benzoyl]amino]ethyl]methylamino]ethyl]amino]carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

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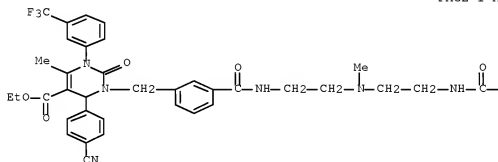
PAGE 1-B



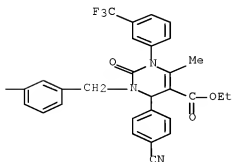
RN 904957-94-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[3-[[[2-[[[2-[[3-[[6-(4-cyanophenyl)-5-(ethoxycarboxyl)yl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]benzoyl]amino]ethyl]methylo]amino]ethyl]amino]carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]phenyl]-, ethyl ester (CA INDEX NAME)

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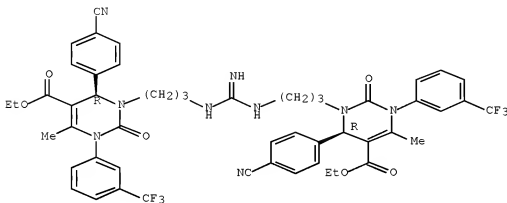
PAGE 1-B



RN 904957-95-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonimidoylbis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

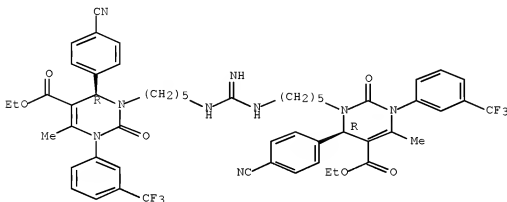
Absolute stereochemistry.



RN 904957-96-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonimidoylbis(imino-5,1-pentanediy)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

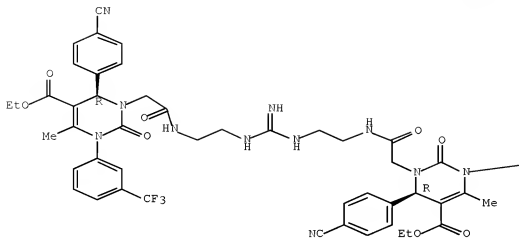


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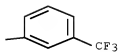
CN 5-Pyrimidinecarboxylic acid, 1,1'-(7-imino-2,12-dioxo-3,6,8,11-tetraaza-1,13-tridecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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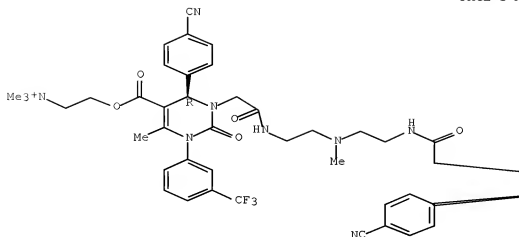


RN 904957-98-8 ZCAPLUS

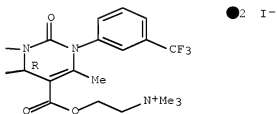
CN Ethanaminium, 2,2'-[(methylimino)bis[2,1-ethanediyylimino(2-oxo-2,1-ethanediy)] [(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1,5(2H)-pyrimidinediy]]carbonyloxy]]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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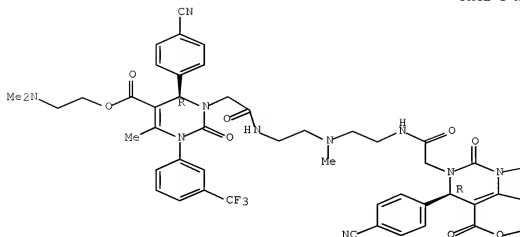


RN 904957-99-9 ZCAPLUS

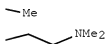
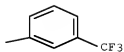
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[[2-[[[2-(6R)-6-(4-cyanophenyl)-5-[[[2-(dimethylamino)ethyl]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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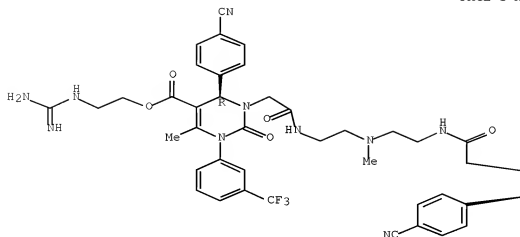
RN 904958-00-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[(6R)-5-[[2-[(aminoiminomethyl)amino]ethoxy]carbonyl]-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(aminoiminomethyl)amino]ethyl ester, (4R)-(CA INDEX NAME)

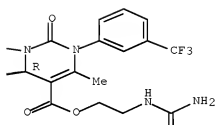
Absolute stereochemistry.



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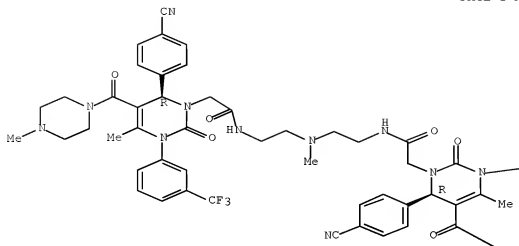
$$\begin{array}{c} \text{U} \\ \text{NH} \end{array}$$

RN 904958-01-6 ZCAPLUS

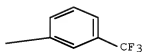
CN 1 (2H)-Pyrimidineacetamide, N,N'-[(methylimino)di-2,1-ethanediy]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[(4-methyl-1-piperazinyl)carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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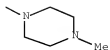


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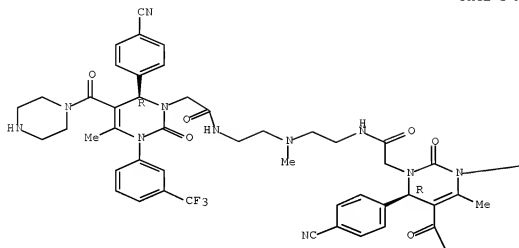


RN 904958-02-7 ZCAPLUS

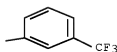
CN 1 (2H)-Pyrimidineacetamide, N,N'-[(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(1-piperazinylcarbonyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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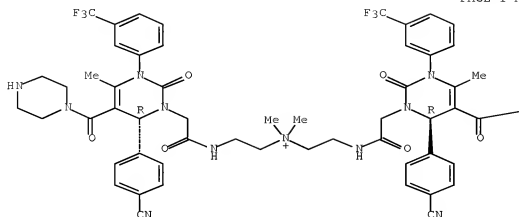
PAGE 2-A



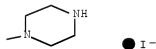
RN	904958-03-8	ZCAPLUS
CN	<p>Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(1-piperazinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(1-piperazinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)</p>	

Absolute stereochemistry.

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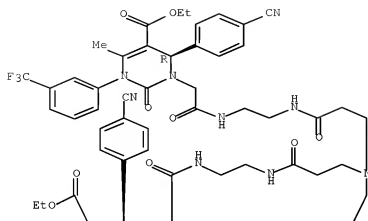


RN 904958-04-9 ZCAPLUS

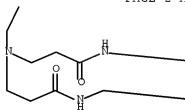
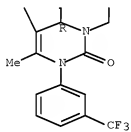
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[22-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]-10,13-bis[3-[[2-[[2-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]amino]-3-oxopropyl]-2,7,16,21-tetraoxo-3,6,10,13,17,20-hexaazadocos-1-yl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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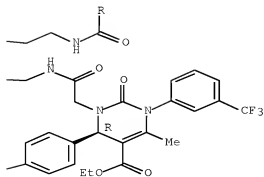


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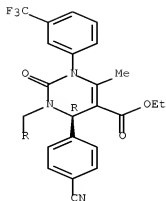


NC

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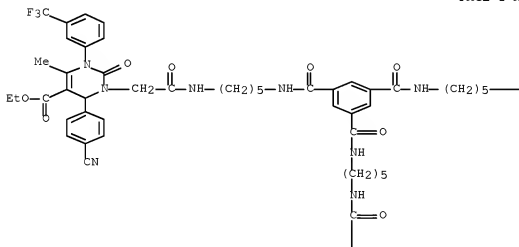


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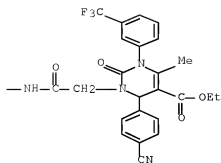


RN 904958-05-0 ZCAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 3-[2-[[[3,5-bis[[[5-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]pentyl]amino]carbo-  
 nyl]benzoyl]amino]pentyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA  
 INDEX NAME)

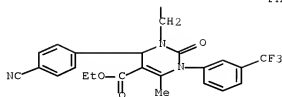
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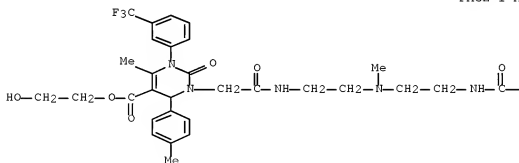
PAGE 2-A



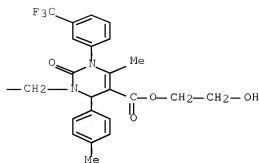
RN 904958-06-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[[2-[3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-6-(4-methylphenyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-4-(4-methylphenyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)

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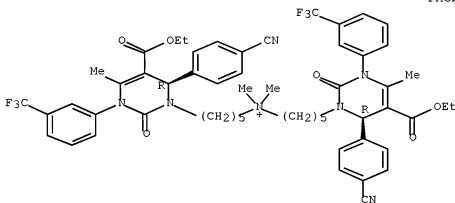


RN 904958-08-3 ZCAPLUS

CN 1(2H)-Pyrimidinepentanaminium, 6-(4-cyanophenyl)-N-[5-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]pentyl]-5-(ethoxycarbonyl)-3,6-dihydro-N,N,4-trimethyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, iodide (1:1), (6R)- (CA INDEX NAME)

Absolute stereochemistry.

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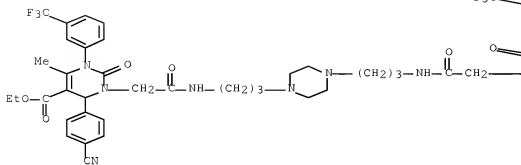


RN 904958-09-4 ZCAPLUS

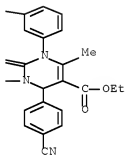
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[3-[4-[3-[[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]propyl]-1-piperazinyl]propyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



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F<sub>3</sub>C

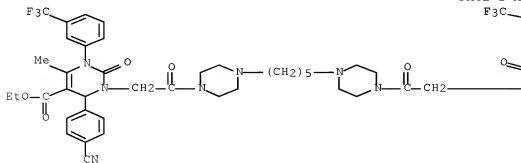
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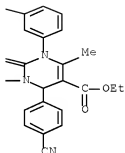
RN 904958-10-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[4-[5-[4-[2-[6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]-1-piperazinyl]pentyl]-1-piperazinyl]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

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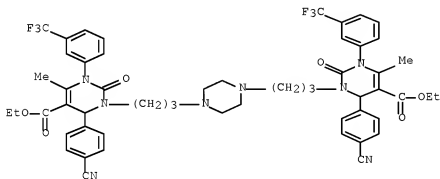
F<sub>3</sub>C

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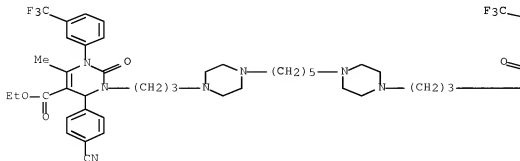
RN 904958-11-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,4-piperazinediyl-di-3,1-propanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904958-12-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,5-pentanediyldi-bis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



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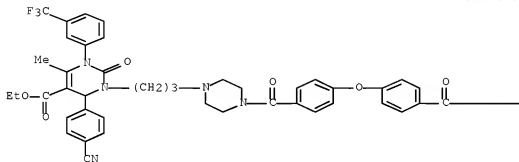
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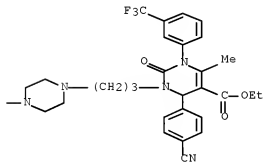
RN 904958-14-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[oxybis(4,1-phenylenecarbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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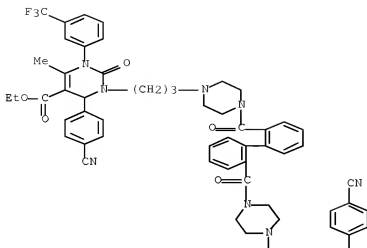
PAGE 1-B



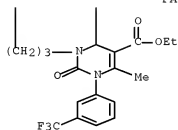
RN 904958-15-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[[1,1'-biphenyl]-2,2'-diylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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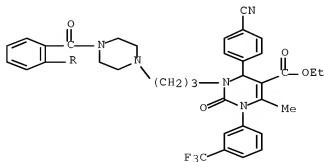


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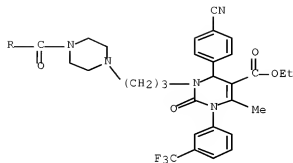


RN 904958-16-3 ZCAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-phenylenebis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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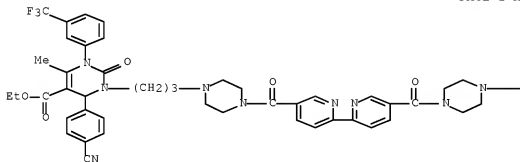
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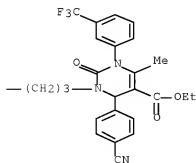
RN 904958-17-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[[2,2'-bipyridin]-5,5'-diylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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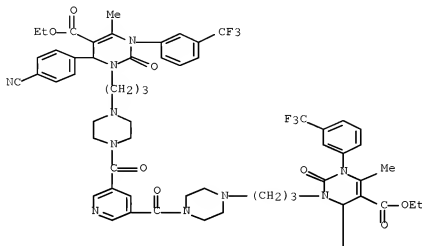
PAGE 1-B



RN 904958-18-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[3,5-pyridinediylbis(carbonyl-4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

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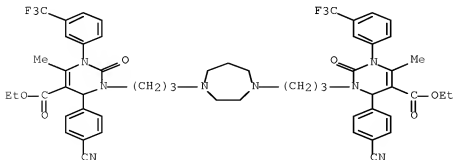


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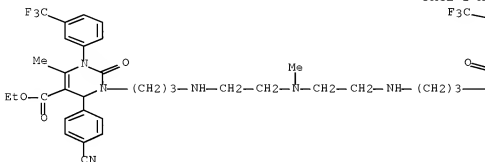
RN 904958-19-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(tetrahydro-1H-1,4-diazepine-1,4(5H)-diyl)di-3,1-propanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 904958-20-9 ZCAPLUS

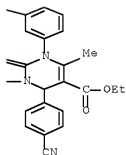
CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)bis(2,1-ethanediylimino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



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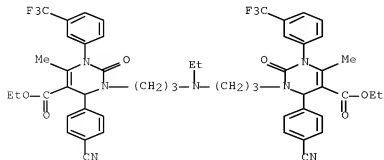
F<sub>3</sub>C

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RN 904958-21-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)



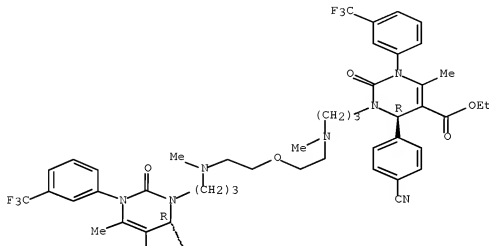


RN 904958-22-1 ZCAPLUS

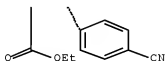
CN 5-Pyrimidinecarboxylic acid, 1,1'-[oxybis[2,1-ethanediyl(methylimino)-3,1-propanediyl]]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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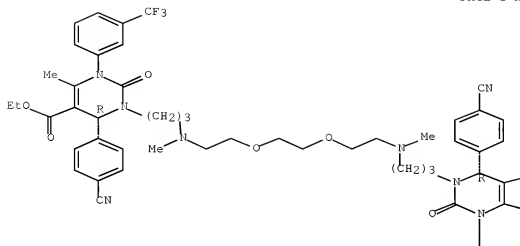


RN 904958-23-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(4,13-dimethyl-7,10-dioxo-4,13-diazahexadecane-1,16-diyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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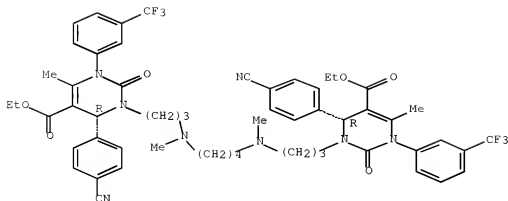
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RN 904958-24-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,4-butanediylbis[(methylimino)-3,1-propanediyl]]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

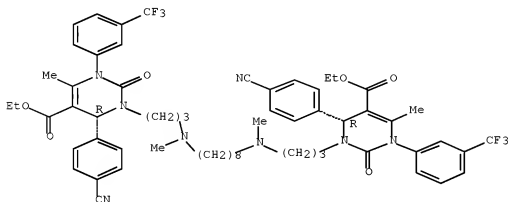
Absolute stereochemistry.



RN 904958-25-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,8-octanediylbis[(methylimino)-3,1-propanediyl]]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

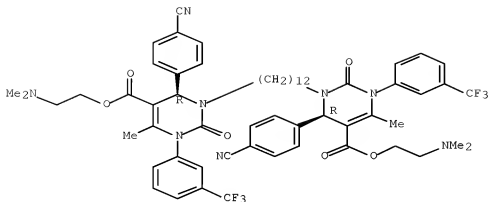


RN 904958-26-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[(methylimino)di-2,1-ethanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





RN 904958-30-1 ZCAPLUS

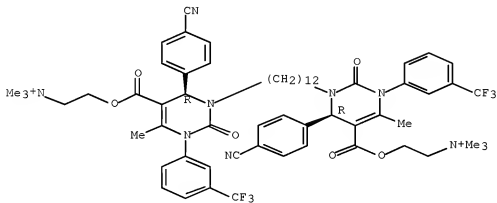
CN Ethanaminium, 2-[[[(4R)-4-(4-cyanophenyl)-3-[12-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-5-[2-(trimethylammonio)ethoxy]carbonyl]-1(2H)-pyrimidinyl]dodecyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyloxy]-N,N,N-trimethyl-, formate (1:2) (CA INDEX NAME)

CM 1

CRN 904958-29-8

CMF C62 H74 F6 N8 O6

Absolute stereochemistry.



CM 2

CRN 71-47-6

CMF C H O2

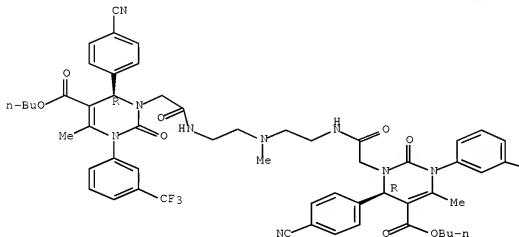
O=CH-O-

RN 904958-31-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[(6R)-5-(butoxycarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, butyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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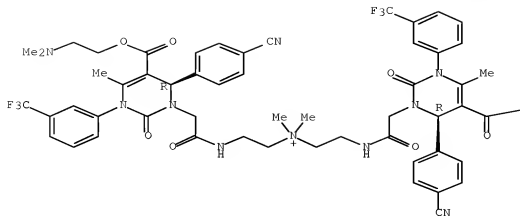
—CF<sub>3</sub>

RN 904958-32-3 ZCAPLUS

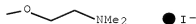
CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-5-[[2-(dimethylamino)ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-5-[[2-(dimethylamino)ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B

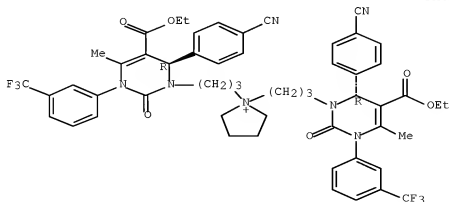


RN 904958-33-4 ZCAPLUS

CN Pyrrolidinium, 1,1-bis[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



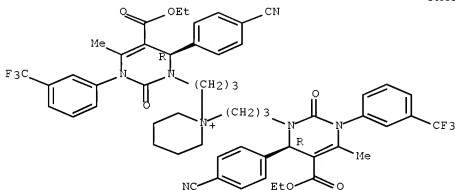
PAGE 2-A



RN 904958-34-5 ZCAPLUS  
 CN Piperidinium, 1,1-bis[3-[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]propyl]-, bromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

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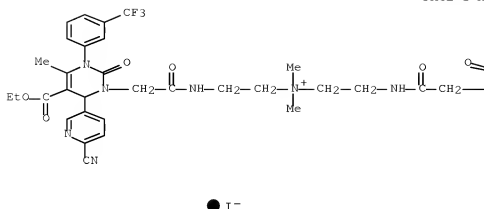
PAGE 2-A



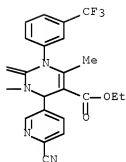
RN 904958-36-7 ZCAPLUS  
 CN Ethanaminium, 2-[[2-[6-(6-cyano-3-pyridinyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[6-(6-cyano-3-pyridinyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)



PAGE 1-A



PAGE 1-B

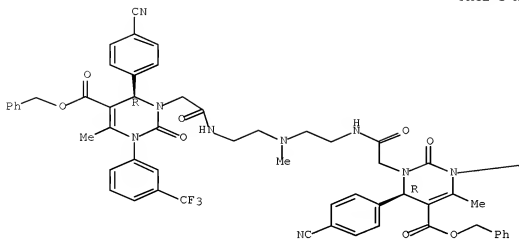


RN 904958-37-8 ZCAPLUS

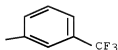
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, phenylmethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B



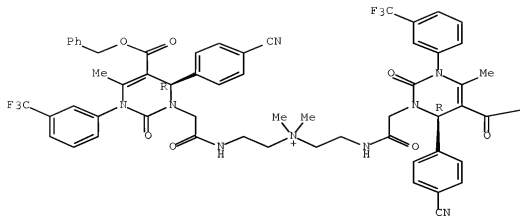
RN 904958-39-0 ZCAPLUS  
 CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-  
 [(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-  
 pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-  
 methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-  
 1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, formate (1:1) (CA  
 INDEX NAME)

CM 1

CRN 904958-38-9  
 CMF C64 H58 F6 N9 O8

Absolute stereochemistry.

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CM 2

CRN 71-47-6

CMF C H O2



RN 904958-41-4 ZCAPLUS

CN Ethanaminium, 2-[[[[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[[[(6R)-6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, butanedioate (2:1) (9CI) (CA INDEX NAME)

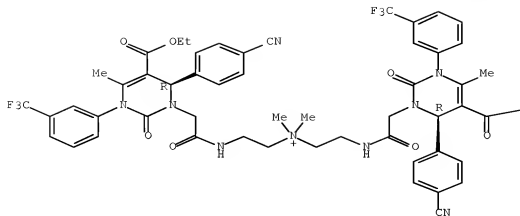
CM 1

CRN 904958-40-3

CMF C54 H54 F6 N9 O8

Absolute stereochemistry.

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—OEt

CM 2

CRN 56-14-4

CMF C4 H4 O4

-O<sub>2</sub>C—CH<sub>2</sub>—CH<sub>2</sub>—CO<sub>2</sub>-

IT 904958-45-8P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of multimers of tetrahydropyrimidinone compds.)

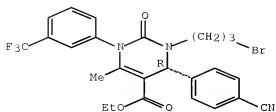
as

elastase inhibitors useful in the treatment of respiratory diseases)

RN 904958-45-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 904958-43-6P 904958-44-7P 904958-46-9P  
 904958-47-0P 904958-48-1P 904958-49-2P  
 904958-51-6P 904958-52-7P 904958-53-8P  
 904958-54-9P 904958-55-0P 904958-56-1P  
 904958-57-2P 904958-58-3P 904958-59-4P  
 904958-60-7P 904958-61-8P 904958-62-9P  
 904958-63-0P 904958-64-1P 904958-65-2P  
 904958-66-3P 904958-67-4P 904958-68-5P  
 904958-69-6P 904958-70-9P 904958-71-0P  
 904958-72-1P 904958-75-4P 904958-76-5P  
 904958-77-6P 904958-79-8P 904958-80-1P  
 904958-81-2P 904958-83-4P 904958-97-0P  
 904958-98-1P 904958-99-2P 904959-00-8P  
 904959-02-1P 904959-04-2P 904959-05-3P  
 904959-06-1P 904959-06-6P 904959-16-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of multimers of tetrahydropyrimidinone compds.

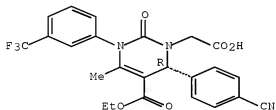
as

elastase inhibitors useful in the treatment of respiratory diseases)

RN 904958-43-6 ZCAPLUS

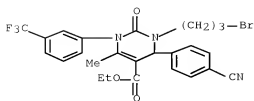
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



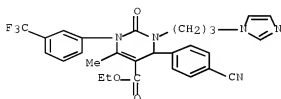
RN 904958-44-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-46-9 ZCAPLUS

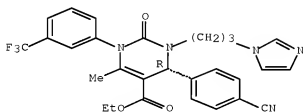
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[3-(1H-imidazol-1-yl)propyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-47-0 ZCAPLUS

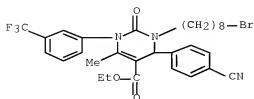
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[3-(1H-imidazol-1-yl)propyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 904958-48-1 ZCAPLUS

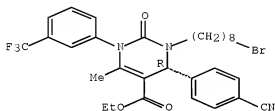
CN 5-Pyrimidinecarboxylic acid, 3-(8-bromooctyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-49-2 ZCAPLUS

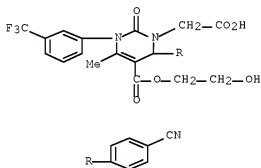
CN 5-Pyrimidinecarboxylic acid, 3-(8-bromooctyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 904958-51-6 ZCAPLUS

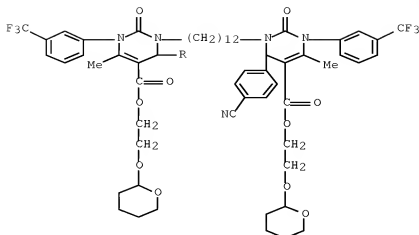
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-[(2-hydroxyethoxy)carbonyl]-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



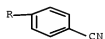
RN 904958-52-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-(1,12-dodecanediyl)bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl] ester (9CI) (CA INDEX NAME)

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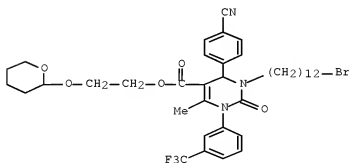


PAGE 2-A



RN 904958-53-8 ZCAPLUS

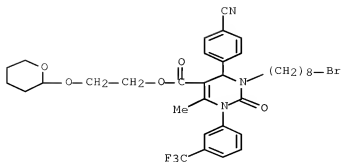
CN 5-Pyrimidinecarboxylic acid, 3-(12-bromododecyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



RN 904958-54-9 ZCAPLUS

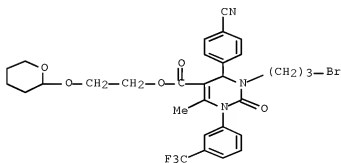
CN 5-Pyrimidinecarboxylic acid, 3-(8-bromooctyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)





RN 904958-55-0 ZCAPLUS

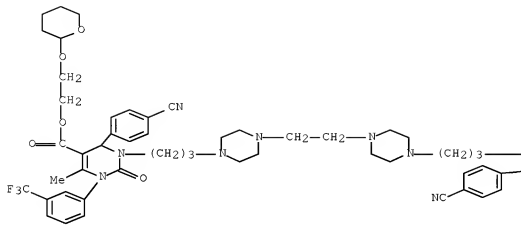
CN 5-Pyrimidinecarboxylic acid, 3-(3-bromopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl ester (CA INDEX NAME)



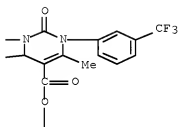
RN 904958-56-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[1,2-ethanediylbis(4,1-piperazinediyl-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl] ester (9CI) (CA INDEX NAME)

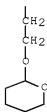
PAGE 1-A



PAGE 1-B

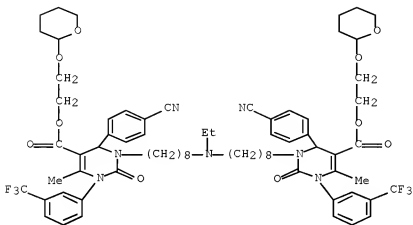


PAGE 2-B



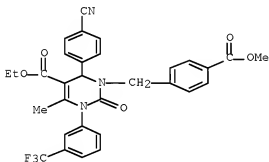
RN 904958-57-2 ZCAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 1,1'-[(ethylimino)di-8,1-octanediyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-

(trifluoromethyl)phenyl]-, bis[2-[(tetrahydro-2H-pyran-2-yl)oxy]ethyl]  
ester (9CI) (CA INDEX NAME)



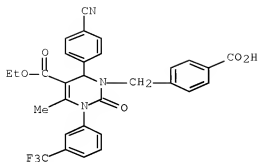
RN 904958-58-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[[4-(methoxycarbonyl)phenyl]methyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



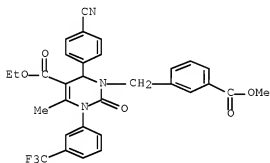
RN 904958-59-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(4-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)



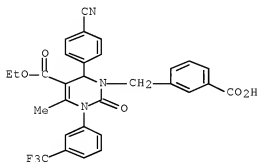
RN 904958-60-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[[3-(methoxycarbonyl)phenyl]methyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-61-8 ZCAPLUS

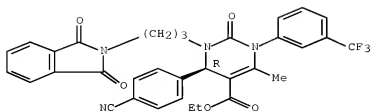
CN 5-Pyrimidinecarboxylic acid, 3-[[3-(3-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)



RN 904958-62-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

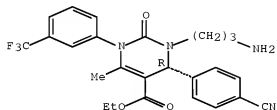
Absolute stereochemistry.



RN 904958-63-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(3-aminopropyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

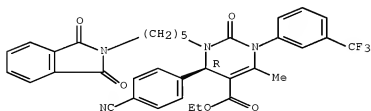
Absolute stereochemistry.



RN 904958-64-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[5-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)pentyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

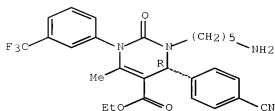
Absolute stereochemistry.



RN 904958-65-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(5-aminopentyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

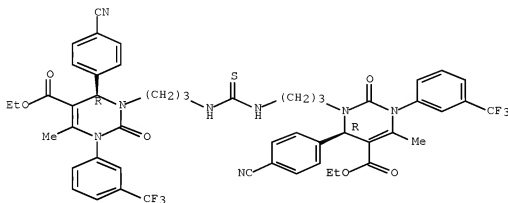
Absolute stereochemistry.



RN 904958-66-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonothioylbis(imino-3,1-propanediyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

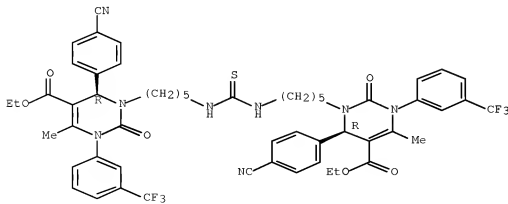
Absolute stereochemistry.



RN 904958-67-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,1'-[carbonothioylbis(imino-5,1-pentanedyl)]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

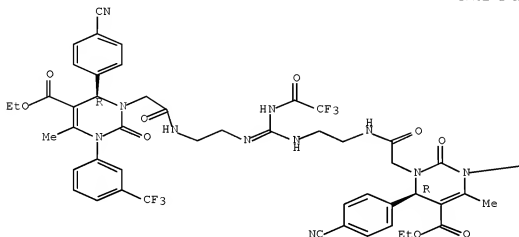


RN 904958-68-5 ZCAPLUS

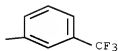
CN 5-Pyrimidinecarboxylic acid, 1,1'-[2,12-dioxo-7-[(trifluoroacetyl)amino]-3,6,8,11-tetraaza-6-tridecene-1,13-diyl]bis[6-(4-cyanophenyl)-1,2,3,6-tetrahydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, diethyl ester, (6R,6'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



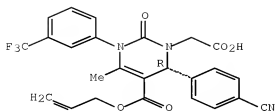
PAGE 1-B



RN 904958-69-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.

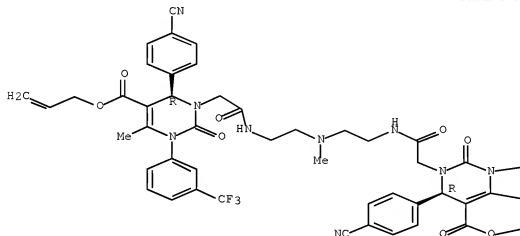


RN 904958-70-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl)methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester, (4R)- (CA INDEX NAME)

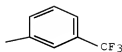
Absolute stereochemistry.

PAGE 1-A





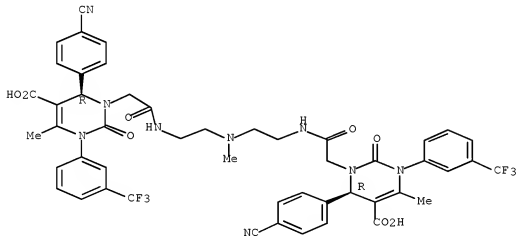
PAGE 1-B



RN 904958-71-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[[2-[[2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

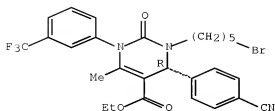
Absolute stereochemistry.



RN 904958-72-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(5-bromopentyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

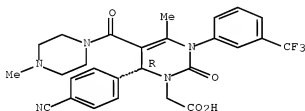
Absolute stereochemistry.



RN 904958-75-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[(4-methyl-1-piperazinyl)carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

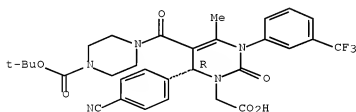
Absolute stereochemistry.



RN 904958-76-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.

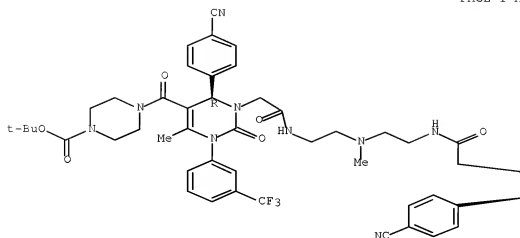


RN 904958-77-6 ZCAPLUS

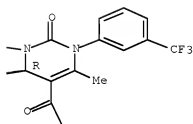
CN 1-Piperazinecarboxylic acid, 4-[[[(4R)-4-(4-cyanophenyl)-3-[2-[2-[2-[(6R)-6-(4-cyanophenyl)-5-[[4-[(1,1-dimethylethoxy)carbonyl]-1-piperazinyl]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-5-pyrimidinyl]carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

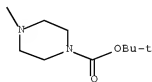
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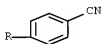
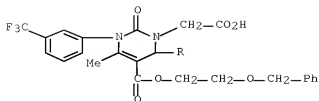
PAGE 1-B



PAGE 2-B



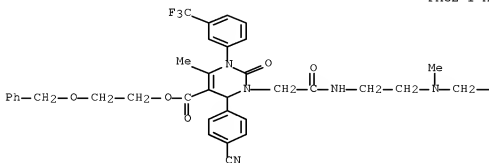
RN 904958-79-8 ZCAPLUS  
 CN 1-(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-  
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 INDEX NAME)



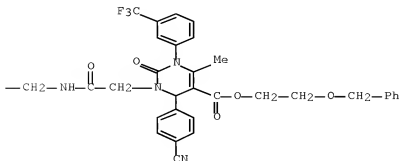
RN 904958-80-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[2-[[2-[[2-(6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(phenylmethoxy)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]methylamino]ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(phenylmethoxy)ethyl ester (CA INDEX NAME)

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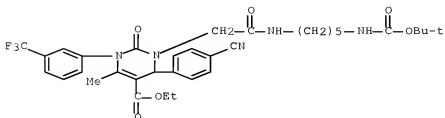


PAGE 1-B



RN 904958-81-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[5-[[[(1,1-dimethylethoxy)carbonyl]amino]pentyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



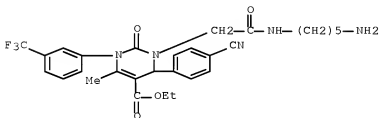
RN 904958-83-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[2-[(5-aminopentyl)amino]-2-oxoethyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 904958-82-3

CMF C29 H32 F3 N5 O4



CM 2

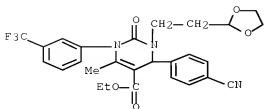
CRN 76-05-1

CMF C2 H F3 O2



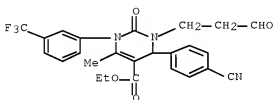
RN 904958-97-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(1,3-dioxolan-2-yl)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-98-1 ZCAPLUS

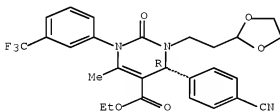
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 904958-99-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(1,3-dioxolan-2-yl)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

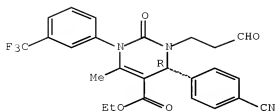
Absolute stereochemistry.



RN 904959-00-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (4R)- (CA INDEX NAME)

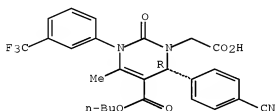
Absolute stereochemistry.



RN 904959-03-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(butoxycarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

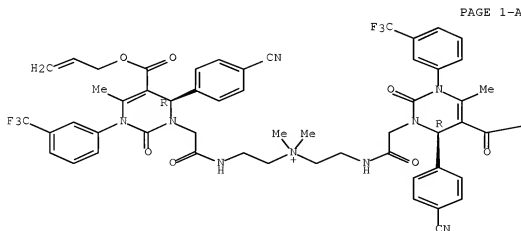
Absolute stereochemistry.



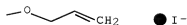
RN 904959-04-2 ZCAPLUS

CN Ethanaminium, 2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.



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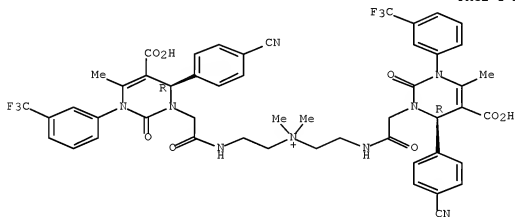


RN 904959-05-3 ZCAPLUS

CN Ethanaminium, 2-[[2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-N-[2-[[2-[(6R)-5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]ethyl]-N,N-dimethyl-, iodide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

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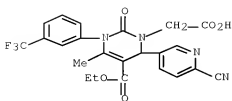
PAGE 2-A



RN 904959-06-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(6-cyano-3-pyridinyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

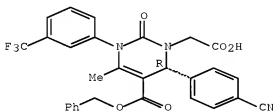




RN 904959-08-6 ZCAPLUS

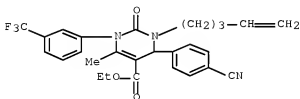
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(phenylmethoxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 904959-16-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(4-penten-1-yl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



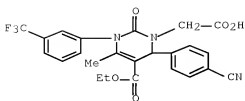
IT 671776-27-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of multimers of tetrahydropyrimidinone compds. as elastase inhibitors useful in the treatment of respiratory diseases)

RN 671776-27-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L6 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:979623 ZCAPLUS Full-text  
 DOCUMENT NUMBER: 143:286441  
 TITLE: Preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors  
 INVENTOR(S): Gielen-Haertwig, Heike; Albrecht, Barbara; Keldenich, Joerg; Li, Volkhart; Pernerstorfer, Josef; Schlemmer, Karl-Heinz; Telan, Leila  
 PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany  
 SOURCE: PCT Int. Appl., 141 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082864	A1	20050909	WO 2005-EP1486	20050215
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2557271	A1	20050909	CA 2005-2557271	20050215
EP 1723121	A1	20061122	EP 2005-707386	20050215
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JP 2007524696	T	20070830	JP 2007-500099	20050215
US 20080064704	A1	20080313	US 2007-590770	20070618
PRIORITY APPLN. INFO.:			EP 2004-4314	A 20040226
			WO 2005-EP1486	W 20050215
OTHER SOURCE(S):		CASREACT 143:286441; MARPAT 143:286441		
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [A = aryl or heteroaryl ring; R1, R2 and R3 independently = H, halo, nitro, etc.; R4 = (un)substituted alkyl, cycloalkylcarbonyl,

alkylcarbonyl, etc.; R5 = (un)substituted alkyl; R6 = H, formyl, aminocarbonyl, etc.; R7 = cyano, OH, nitro, etc.; V, W, X, Y and Z independently = CH or N wherein the ring contains either 0, 1 or 2 nitrogen atoms} and their pharmaceutically acceptable salts, are prepared and disclosed as human neutrophil elastase (HNE) inhibitors. Thus, e.g., II was prepared by cyclization of N-[3-(trifluoromethyl)phenyl]urea and 4-cyanobenzaldehyde with ethyl-3-oxobutanoate and subsequent reduction using LAH. The activity of I against HNE was evaluated in an in vitro enzyme assay utilizing a fluorogenic peptide substrate and it was revealed that selected compds. of the invention possessed IC50 values in the range of 5 up to 1000 nM. I as inhibitors of human neutrophil elastase should prove useful in the treatment of chronic obstructive pulmonary diseases, acute coronary syndrome, acute myocardial infarction and heart failure development. Pharmaceutical compns. comprising I are disclosed.

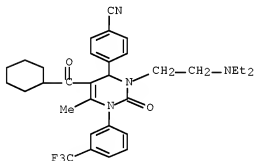
IT 964251-32-1P 864251-33-2P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors)

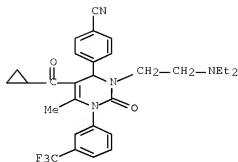
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CN Benzonitrile, 4-[5-(cyclohexylcarbonyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]-(CA INDEX NAME)



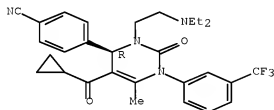
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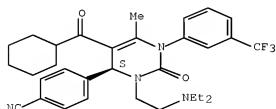
IT 864251-36-5P 864251-37-6P  
 RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN  
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); USES (Uses)  
 (preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase  
 inhibitors)  
 RN 864251-36-5 ZCAPLUS  
 CN Benzonitrile, 4-[(4R)-5-(cyclopropylcarbonyl)-3-[2-(diethylamino)ethyl]-  
 1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-  
 pyrimidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 864251-37-6 ZCAPLUS  
 CN Benzonitrile, 4-[(4S)-5-(cyclohexylcarbonyl)-3-[2-(diethylamino)ethyl]-  
 1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-  
 pyrimidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



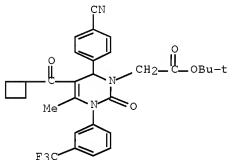
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 864250-75-9P 864250-78-2P 864250-82-8P

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 864251-24-1P 864251-27-4P 864251-29-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase inhibitors)

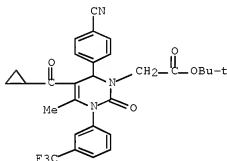
RN 864250-66-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



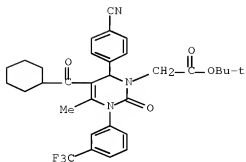
RN 864250-67-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



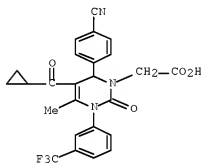
RN 864250-68-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



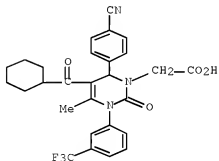
RN 864250-71-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



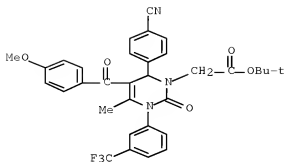
RN 864250-72-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



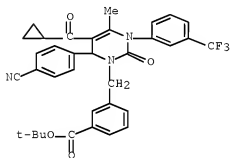
RN 864250-73-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(4-methoxybenzoyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



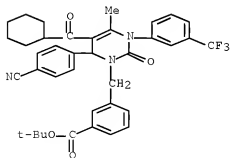
RN 864250-75-9 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



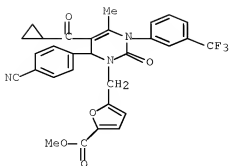
RN 864250-78-2 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



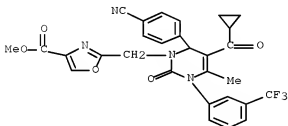
RN 864250-82-8 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



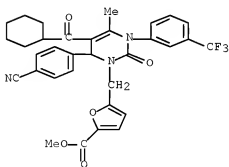
RN 864250-83-9 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864250-86-2 ZCAPLUS

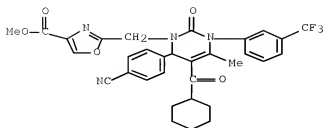
CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864250-87-3 ZCAPLUS

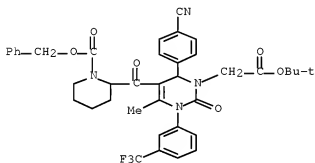
CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)





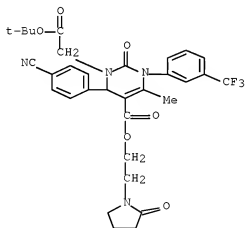
RN 864250-95-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[1-[(phenylmethoxy)carbonyl]-2-piperidinyl]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-05-8 ZCAPLUS

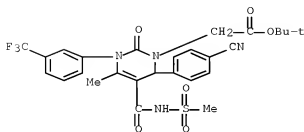
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(2-oxo-1-pyrrolidinyl)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-08-1 ZCAPLUS

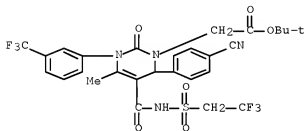
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[[2-(2-oxo-1-pyrrolidinyl)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

1,1-dimethylethyl ester (CA INDEX NAME)



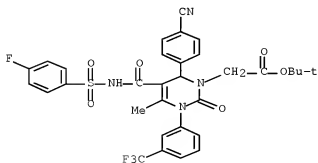
RN 864251-09-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[[(2,2,2-trifluoroethyl)sulfonyl]amino]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



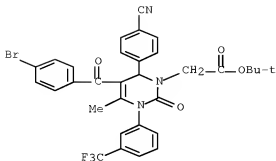
RN 864251-10-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[[(4-fluorophenyl)sulfonyl]amino]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



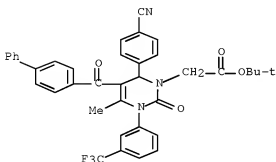
RN 864251-22-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(4-bromobenzoyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



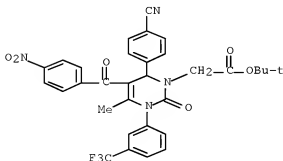
RN 864251-24-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-([1,1'-biphenyl]-4-ylcarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-27-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(4-nitrobenzoyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

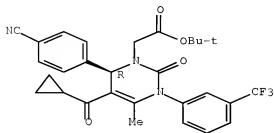


RN 864251-29-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

ester, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



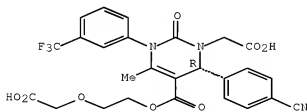
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 864250-88-4F 864250-89-5P 864250-90-6P  
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 864251-04-7P 864251-06-9P 864251-07-0P  
 864251-14-9P 864251-15-0P 864251-16-1P  
 864251-17-2P 864251-23-0P 864251-25-2P  
 864251-28-5P 864251-30-9P 864251-34-3P  
 864251-35-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)  
 (preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase  
 inhibitors)

RN 864250-45-3 ZCAPLUS

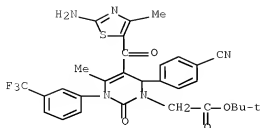
CN 1(2H)-Pyrimidineacetic acid, 5-[[2-(carboxymethoxy)ethoxy]carbonyl]-6-(4-  
 cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-,  
 (6R)- (CA INDEX NAME)

Absolute stereochemistry.



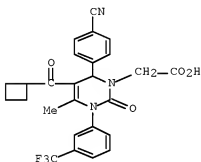
RN 864250-69-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-[(2-amino-4-methyl-5-thiazolyl)carbonyl]-6-  
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 1,1-dimethylethyl ester (CA INDEX NAME)



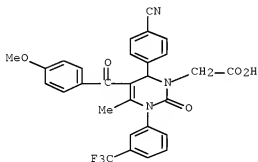
RN 864250-70-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclobutylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



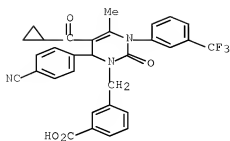
RN 864250-74-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(4-methoxybenzoyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



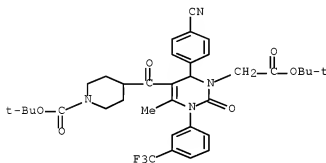
RN 864250-76-0 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



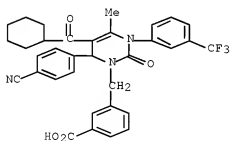
RN 864250-79-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[1-[(1,1-dimethylethoxy)carbonyl]-4-piperidiny]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



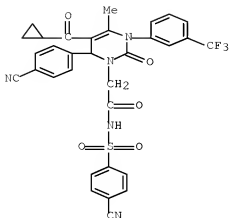
RN 864250-80-6 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



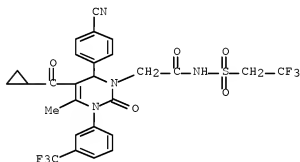
RN 864250-84-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



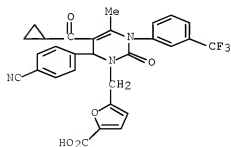
RN 864250-85-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864250-88-4 ZCAPLUS

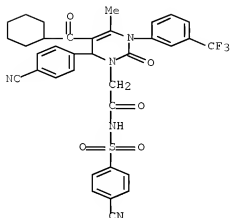
CN 2-Furancarboxylic acid, 5-[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864250-89-5 ZCAPLUS

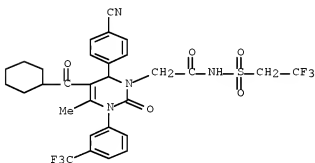
CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



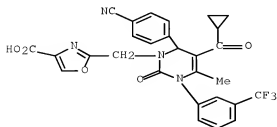
RN 864250-90-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864250-91-9 ZCAPLUS

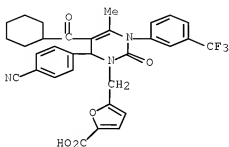
CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)





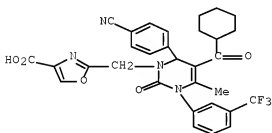
RN 864250-92-0 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



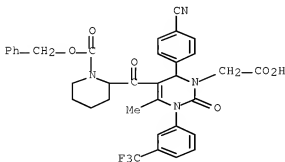
RN 864250-93-1 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(cyclohexylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



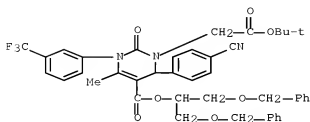
RN 864250-96-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[1-(phenylmethoxy)carbonyl]-2-piperidinyl]carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864251-02-5 ZCAPLUS

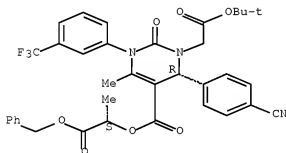
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-(phenylmethoxy)-1-[(phenylmethoxy)methyl]ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-03-6 ZCAPLUS

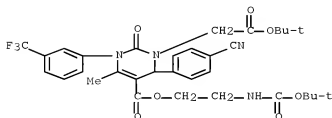
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[[[(1S)-1-methyl-2-oxo-2-(phenylmethoxy)ethoxy]carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)-rel- (CA INDEX NAME)

Relative stereochemistry.



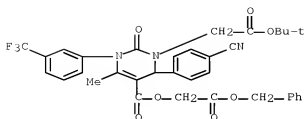
RN 864251-04-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethoxy]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



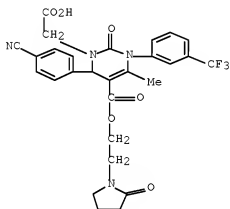
RN 864251-06-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-oxo-2-(phenylmethoxy)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



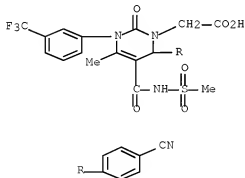
RN 864251-07-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[[2-[(2-oxo-1-pyrrolidinyl)ethoxy]carbonyl]-3-[3-(trifluoromethyl)phenyl]]- (CA INDEX NAME)



RN 864251-14-9 ZCAPLUS

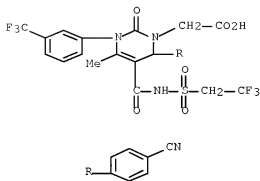
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-[[[(methylsulfonyl)amino]carbonyl]-2-oxo-3-[3-(trifluoromethyl)phenyl]]- (CA INDEX NAME)



RN 864251-15-0 ZCAPLUS

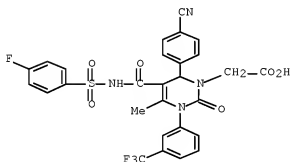
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-

5-[[[(2,2,2-trifluoroethyl)sulfonyl]amino]carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



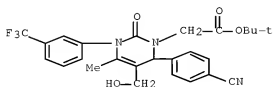
RN 864251-16-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[[[(4-fluorophenyl)sulfonyl]amino]carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



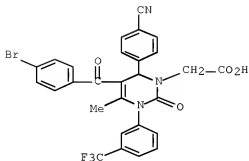
RN 864251-17-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(hydroxymethyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



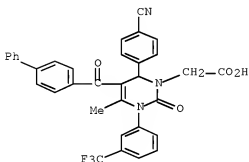
RN 864251-23-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(4-bromobenzoyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



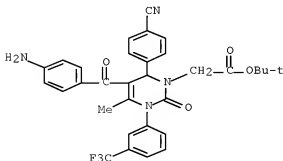
RN 864251-25-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-((1,1'-biphenyl)-4-ylcarbonyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864251-28-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-(4-aminobenzoyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

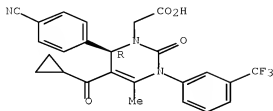


RN 864251-30-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(cyclopropylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

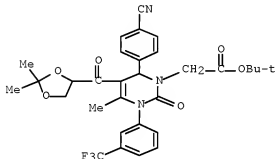
(NAME)

Absolute stereochemistry.



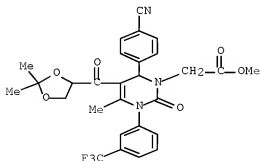
RN 864251-34-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[(2,2-dimethyl-1,3-dioxolan-4-yl)carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864251-35-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-[(2,2-dimethyl-1,3-dioxolan-4-yl)carbonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, methyl ester (CA INDEX NAME)



IT 864151-39-3P 864251-40-1P 864251-41-2F

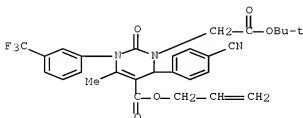
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diaryl-dihydropyrimidin-2-ones as human neutrophil elastase

inhibitors)

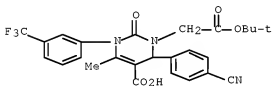
RN 864151-39-3 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



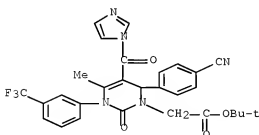
RN 864251-40-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-carboxy-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1-(1,1-dimethylethyl) ester (CA INDEX NAME)



RN 864251-41-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-5-(1H-imidazol-1-ylcarbonyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:979622 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 143:286440

TITLE: Preparation of tetrasubstituted pyrimidin-2-ones as

INVENTOR(S): human neutrophil elastase inhibitors  
 Gielen-Haertwig, Heike; Albrecht, Barbara; Keldenich, Joerg; Li, Volkhart; Pernerstorfer, Josef; Schlemmer, Karl-Heinz; Telan, Leila

PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany

SOURCE: PCT Int. Appl., 119 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

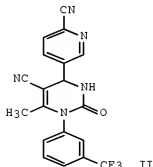
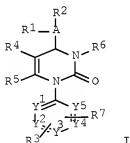
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082863	A2	20050909	WO 2005-EP1487	20050215
WO 2005082863	A3	20051222		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2557272	A1	20050909	CA 2005-2557272	20050215
EP 1730121	A2	20061213	EP 2005-707387	20050215
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2007523931	T	20070823	JP 2007-500100	20050215
US 20080021053	A1	20080124	US 2007-590786	20070720
PRIORITY APPLN. INFO.:			EP 2004-4315	A 20040226
			WO 2005-EP1487	W 20050215

OTHER SOURCE(S): MARPAT 143:286440

GI



AB Title compds. I [A = heteroaryl ring; R1-3 = H, halo, NO2, etc.; R4 = CF3CO, alkylcarbonyl, etc.; R5 = alkyl, alkoxy, etc.; R6 = T-U; T = alkanediyl, akenediyl; U = aryl, heteroaryl, etc.; R7 = halo, NO2, CN, etc.; Y1-5 = independently CH, N wherein the ring contains 0-2 N atoms] and analogs are prepared For instance, II is prepared in 6 steps from 2-bromo-5-



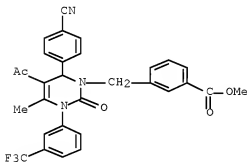
methylpyridine, allyl 3-oxobutanoate and N-[3- (trifluoromethyl)phenyl]urea. II has an IC50 = 70 nM for human neutrophil elastase (HNE). I are useful for the treatment of chronic obstructive pulmonary diseases, acute coronary syndrome, acute myocardial infarction and heart failure development.

IT 864150-42-5P 864150-44-7P 864150-46-9P  
 864150-48-1P 864150-50-5P 864150-52-7P  
 864150-53-8P 864150-54-9P 864150-55-0P  
 864150-56-1P 864150-57-2P 864150-58-3P  
 864150-59-4P 864150-60-7P 864150-61-8P  
 864150-62-9P 864150-63-0P 864150-64-1P  
 864150-61-2P 864150-82-3P 864150-83-4P  
 864150-86-7P 864150-89-0P 864150-93-6P  
 864150-95-8P 864150-97-0P 864151-03-1P  
 864151-05-3P 864151-06-4P 864151-07-5P  
 864151-12-2P 864151-29-1P 864151-50-6P  
 864151-51-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of tetrasubstituted pyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864150-42-5 ZCAPLUS

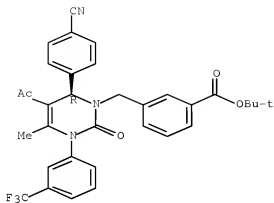
CN Benzoic acid, 3-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-44-7 ZCAPLUS

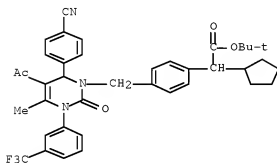
CN Benzoic acid, 3-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



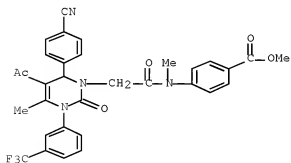
RN 864150-46-9 ZCAPLUS

CN Benzenesacetic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-α-cyclopentyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



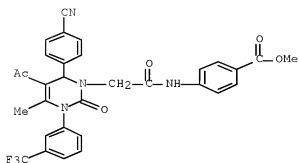
RN 864150-48-1 ZCAPLUS

CN Benzoic acid, 4-[[2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]methylamino]-, methyl ester (CA INDEX NAME)



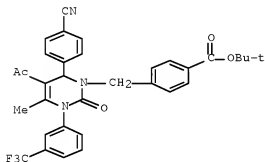
RN 864150-50-5 ZCAPLUS

CN Benzoic acid, 4-[[2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]amino]-, methyl ester (CA INDEX NAME)



RN 864150-52-7 ZCAPLUS

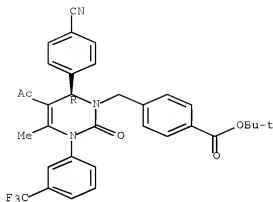
CN Benzoic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864150-53-8 ZCAPLUS

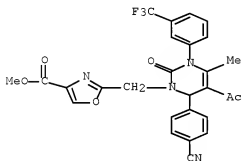
CN Benzoic acid, 4-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-54-9 ZCAPLUS

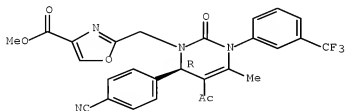
CN 4-Oxazolecarboxylic acid, 2-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-55-0 ZCAPLUS

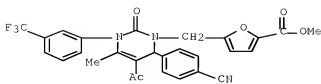
CN 4-Oxazolecarboxylic acid, 2-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-56-1 ZCAPLUS

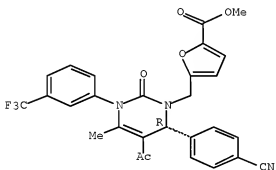
CN 2-Furancarboxylic acid, 5-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-57-2 ZCAPLUS

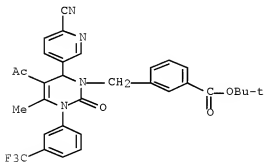
CN 2-Furancarboxylic acid, 5-[[6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



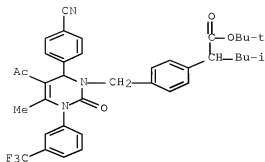
RN 864150-58-3 ZCAPLUS

CN Benzoic acid, 3-[[5-acetyl-6-(6-cyano-3-pyridinyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



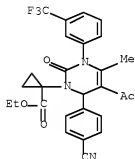
RN 864150-59-4 ZCAPLUS

CN Benzeneacetic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-α-(2-methylpropyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)



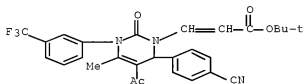
RN 864150-60-7 ZCAPLUS

CN Cyclopropanecarboxylic acid, 1-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]-, ethyl ester (CA INDEX NAME)



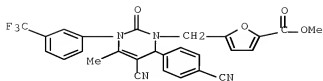
RN 864150-61-8 ZCAPLUS

CN 2-Propenoic acid, 3-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



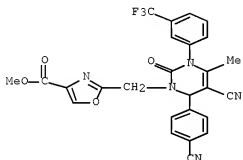
RN 864150-62-9 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



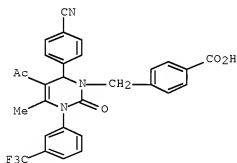
RN 864150-63-0 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



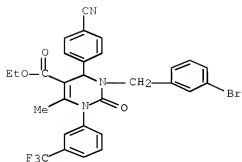
RN 864150-64-1 ZCAPLUS

CN Benzoic acid, 4-[[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



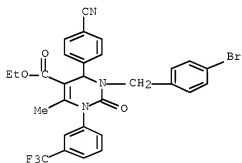
RN 864150-81-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(3-bromophenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 864150-82-3 ZCAPLUS

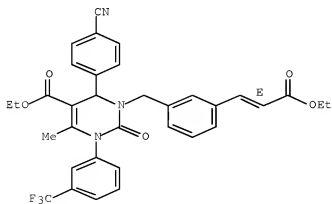
CN 5-Pyrimidinecarboxylic acid, 3-[(4-bromophenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 864150-83-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[3-[(1E)-3-ethoxy-3-oxo-1-propen-1-yl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.

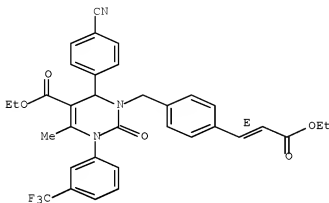


RN 864150-86-7 ZCAPLUS



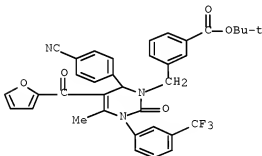
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[4-[(1E)-3-ethoxy-3-oxo-1-propen-1-yl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



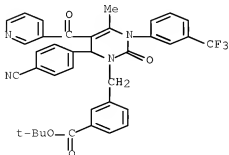
RN 864150-89-0 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



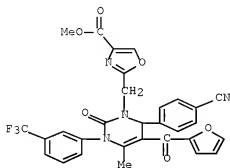
RN 864150-93-6 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



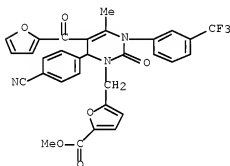
RN 864150-95-8 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864150-97-0 ZCAPLUS

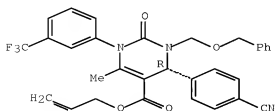
CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



RN 864151-03-1 ZCAPLUS

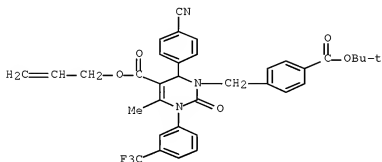
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[(phenylmethoxy)methyl]-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



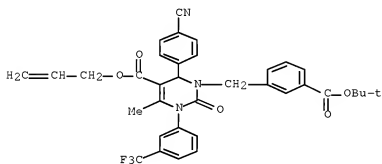
RN 864151-05-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[4-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



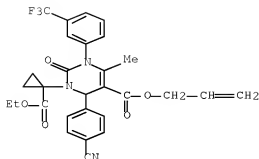
RN 864151-06-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[[3-[(1,1-dimethylethoxy)carbonyl]phenyl]methyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



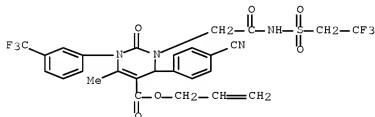
RN 864151-07-5 ZCAPLUS

CN 5(2H)-Pyrimidinecarboxylic acid, 6-(4-cyanophenyl)-1-[1-(ethoxycarbonyl)cyclopropyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



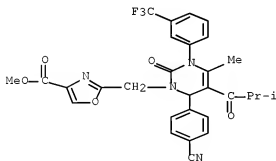
RN 864151-12-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[2-oxo-2-[[2,2,2-trifluoroethyl]sulfonyl]amino]ethyl]-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



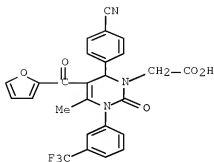
RN 864151-29-1 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



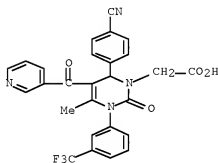
RN 864151-50-8 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-51-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



IT 864150-65-2P 864150-66-3P 864150-67-4P  
 864150-68-5P 864150-69-6P 864150-70-9P  
 864150-71-0P 864150-72-1P 864150-73-2P  
 864150-74-3P 864150-75-4P 864150-76-5P  
 864150-77-6P 864150-78-7P 864150-79-6P  
 864150-80-1P 864150-84-5P 864150-85-6P  
 864150-87-8P 864150-88-9P 864150-90-3P  
 864150-91-4P 864150-92-5P 864150-94-7P  
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 864151-23-5P 864151-24-6P 864151-25-7P  
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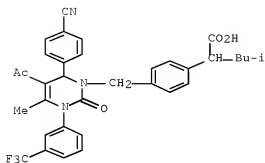
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tetrasubstituted pyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864150-65-2 ZCAPLUS

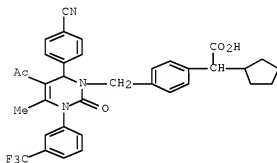
CN Benzeneacetic acid, 4-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-

oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl)methyl]- $\alpha$ -(2-methylpropyl)- (CA INDEX NAME)



RN 864150-66-3 ZCAPLUS

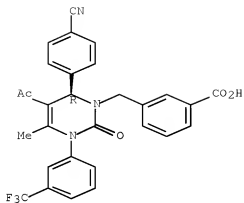
CN Benzoic acid, 4-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl)methyl]-cyclopentyl- (CA INDEX NAME)



RN 864150-67-4 ZCAPLUS

CN Benzoic acid, 3-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl)methyl]- (CA INDEX NAME)

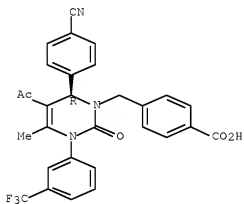
Absolute stereochemistry.



RN 864150-68-5 ZCAPLUS

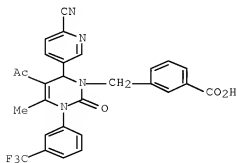
CN Benzoic acid, 4-[[[(6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



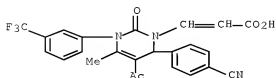
RN 864150-69-6 ZCAPLUS

CN Benzoic acid, 3-[[[5-acetyl-6-(6-cyano-3-pyridinyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



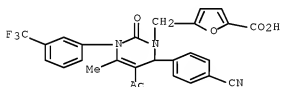
RN 864150-70-9 ZCAPLUS

CN 2-Propenoic acid, 3-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]- (CA INDEX NAME)



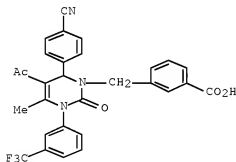
RN 864150-71-0 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864150-72-1 ZCAPLUS

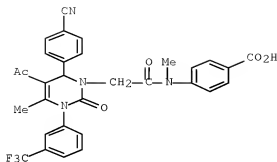
CN Benzoic acid, 3-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864150-73-2 ZCAPLUS

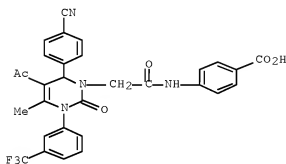
CN Benzoic acid, 4-[[2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl]methylamino]- (CA INDEX NAME)





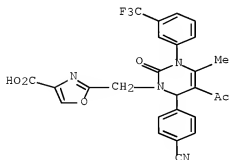
RN 864150-74-3 ZCAPLUS

CN Benzoic acid, 4-[(2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]acetyl)amino]- (CA INDEX NAME)



RN 864150-75-4 ZCAPLUS

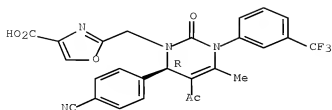
CN 4-Oxazolecarboxylic acid, 2-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864150-76-5 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

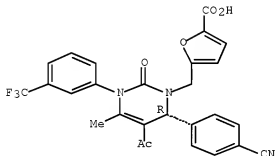
Absolute stereochemistry.



RN 864150-77-6 ZCAPLUS

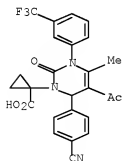
CN 2-Furancarboxylic acid, 5-[[ (6R)-5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-78-7 ZCAPLUS

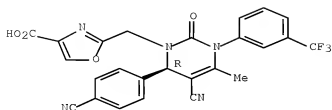
CN Cyclopropanecarboxylic acid, 1-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]- (CA INDEX NAME)



RN 864150-79-8 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[ (6R)-5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)

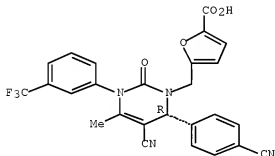
Absolute stereochemistry.



RN 864150-80-1 ZCAPLUS

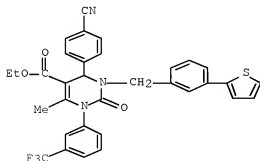
CN 2-Furancarboxylic acid, 5-[[ (6R)-5-cyano-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1 (2H)-pyrimidinyl)methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 864150-84-5 ZCAPLUS

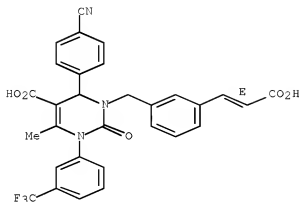
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[[3-(2-thienyl)phenyl)methyl]-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 864150-85-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[[3-[(1E)-2-carboxyethenyl]phenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

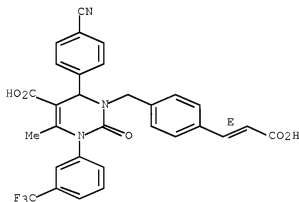
Double bond geometry as shown.



RN 864150-87-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[[4-[(1E)-2-carboxyethenyl]phenyl]methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

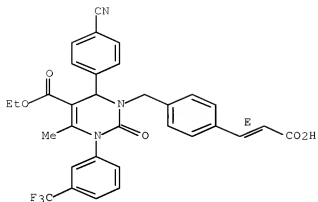
Double bond geometry as shown.



RN 864150-88-9 ZCAPLUS

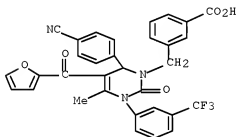
CN 5-Pyrimidinecarboxylic acid, 3-[[4-[(1E)-2-carboxyethenyl]phenyl]methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl ester (CA INDEX NAME)

Double bond geometry as shown.



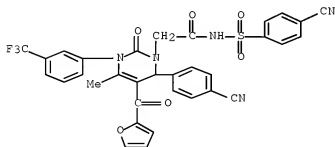
RN 864150-90-3 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



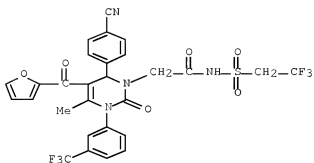
RN 864150-91-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



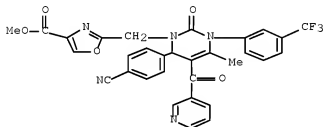
RN 864150-92-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



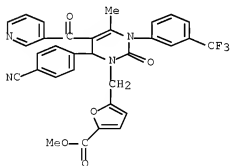
RN 864150-94-7 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



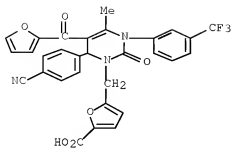
RN 864150-96-9 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]-, methyl ester (CA INDEX NAME)



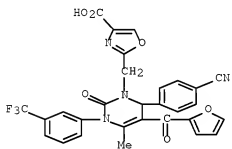
RN 864150-98-1 ZCAPLUS

CN 2-Furancarboxylic acid, 5-[[6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



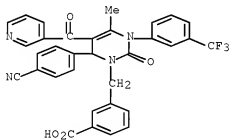
RN 864150-99-2 ZCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-5-(2-furanylicarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



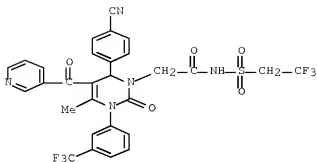
RN 864151-00-8 ZCAPLUS

CN Benzoic acid, 3-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



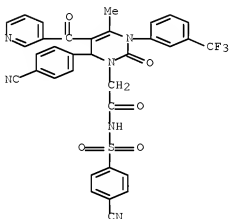
RN 864151-01-9 ZCAPLUS

CN 1-(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-02-0 ZCAPLUS

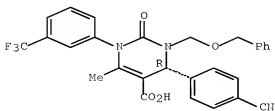
CN 1-(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-04-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[(phenylmethoxy)methyl]-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

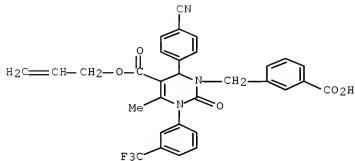


RN 864151-08-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(3-carboxyphenyl)methyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (4R)- (CA INDEX NAME)

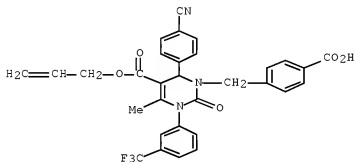


5-(2-propen-1-yl) ester (CA INDEX NAME)



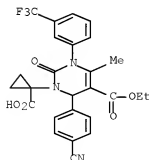
RN 864151-09-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(4-carboxyphenyl)methyl]-4-(4-cyanophenyl)-  
1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-,  
5-(2-propen-1-yl) ester (CA INDEX NAME)



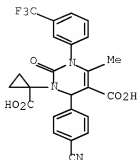
RN 864151-10-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(1-carboxycyclopropyl)-4-(4-cyanophenyl)-  
1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-ethyl  
ester (9CI) (CA INDEX NAME)



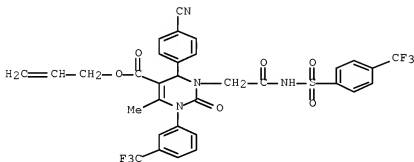
RN 864151-11-1 ZCAPLUS

CN 5(2H)-Pyrimidinecarboxylic acid, 1-(1-carboxycyclopropyl)-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



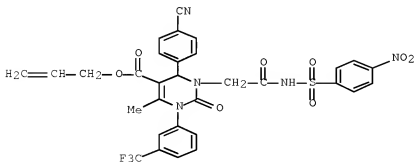
RN 864151-13-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[2-oxo-2-[[[4-(trifluoromethyl)phenyl]sulfonyl]amino]ethyl]-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



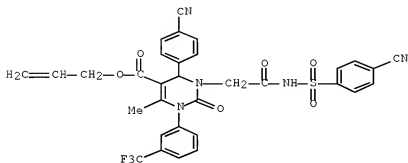
RN 864151-14-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-[[[4-(nitrophenyl)sulfonyl]amino]-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



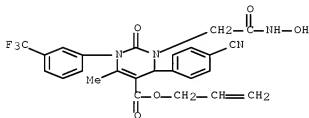
RN 864151-15-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[4-(cyanophenyl)sulfonyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



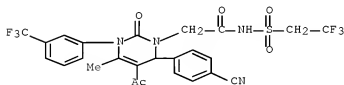
RN 864151-16-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[2-(hydroxyamino)-2-oxoethyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



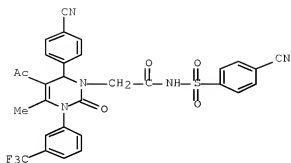
RN 864151-17-7 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-18-8 ZCAPLUS

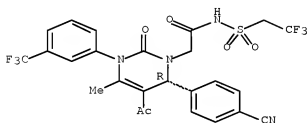
CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-N-[(4-(cyanophenyl)sulfonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-19-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

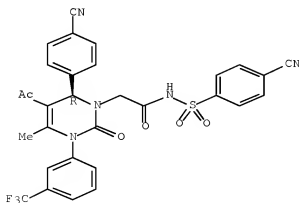
Absolute stereochemistry.



RN 864151-20-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 5-acetyl-6-(4-cyanophenyl)-N-[(4-cyanophenyl)sulfonyl]-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

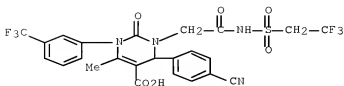
Absolute stereochemistry.



RN 864151-21-3 ZCAPLUS

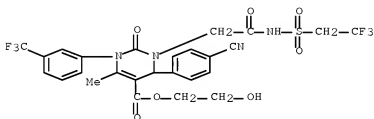
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-

2-oxo-3-[2-oxo-2-[[ (2,2,2-trifluoroethyl)sulfonyl]amino]ethyl]-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



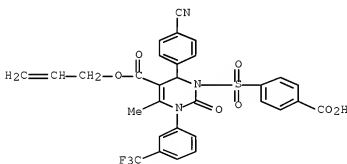
RN 864151-22-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-[2-oxo-2-[[ (2,2,2-trifluoroethyl)sulfonyl]amino]ethyl]-1-[3-(trifluoromethyl)phenyl]-, 2-hydroxyethyl ester (CA INDEX NAME)



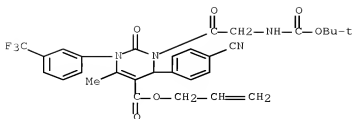
RN 864151-23-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-[(4-carboxyphenyl)sulfonyl]-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 5-(2-propen-1-yl) ester (CA INDEX NAME)



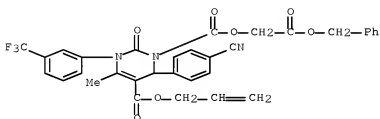
RN 864151-24-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[[ (1,1-dimethylethoxy)carbonyl]amino]acetyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-propen-1-yl ester (CA INDEX NAME)



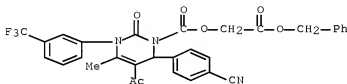
RN 864151-25-7 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1-[2-oxo-2-(phenylmethoxy)ethyl] 5-(2-propen-1-yl) ester (CA INDEX NAME)



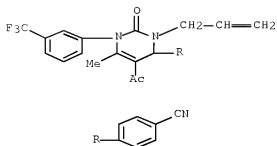
RN 864151-26-8 ZCAPLUS

CN 1(2H)-Pyrimidinedicarboxylic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 2-oxo-2-(phenylmethoxy)ethyl ester (CA INDEX NAME)



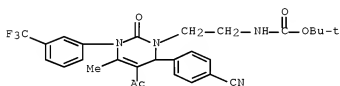
RN 864151-27-9 ZCAPLUS

CN Benzonitrile, 4-[5-acetyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(2-propen-1-yl)-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]- (CA INDEX NAME)



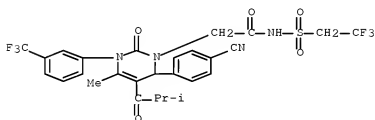
RN 864151-28-0 ZCAPLUS

CN Carbamic acid, [2-[5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



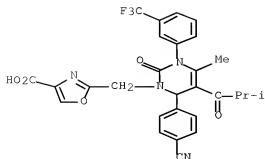
RN 864151-30-4 ZCAPLUS

CN 1(2H)-Pyrimidineacetamide, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-N-[(2,2,2-trifluoroethyl)sulfonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-31-5 ZCAPLUS

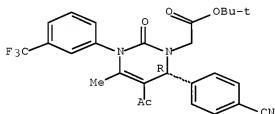
CN 4-Oxazolecarboxylic acid, 2-[[6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-1(2H)-pyrimidinyl]methyl]- (CA INDEX NAME)



RN 864151-49-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 864151-36-2P 864151-39-3P 864151-40-6P

864151-41-7P 864151-42-6P 864151-43-9P

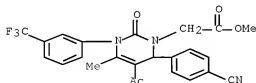
864151-44-0P 864151-45-1P 864151-46-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetrasubstituted pyrimidin-2-ones as human neutrophil elastase inhibitors)

RN 864151-38-2 ZCAPLUS

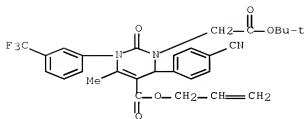
CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, methyl ester (CA INDEX NAME)



RN 864151-39-3 ZCAPLUS

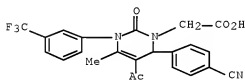
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)





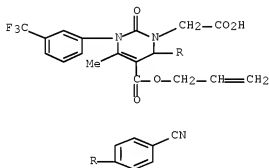
RN 864151-40-6 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-41-7 ZCAPLUS

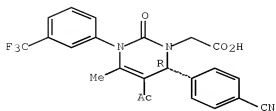
CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-[(2-propen-1-yloxy)carbonyl]-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 864151-42-8 ZCAPLUS

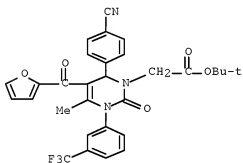
CN 1(2H)-Pyrimidineacetic acid, 5-acetyl-6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, (6R)- (CA INDEX NAME)

Absolute stereochemistry.



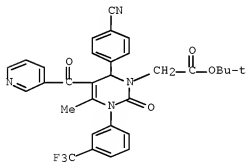
RN 864151-43-9 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(2-furanylcarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



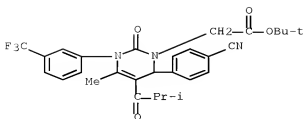
RN 864151-44-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-5-(3-pyridinylcarbonyl)-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



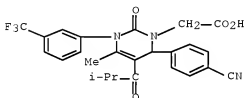
RN 864151-45-1 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 864151-46-2 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-5-(2-methyl-1-oxopropyl)-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



L6 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:253147 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:287406

TITLE: Preparation of pyrimidinones as human neutrophil

elastase (HNE) inhibitors

INVENTOR(S): Gielen, Heike; Li, Volkhart; Rosentreter, Ulrich; Schlemmer, Karl-heinz; Allerheiligen, Swen; Telan, Leila; Baerfacker, Lars; Keldenich, Joerg; Fitzgerald, Mary F.; Nash, Kevin; Albrecht, Barbara; Meurer, Dirk Bayer Healthcare Ag, Germany

SOURCE: PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

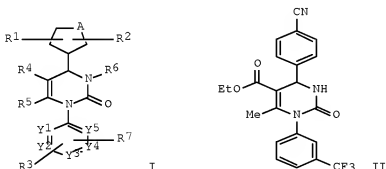
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004024700	A1	20040325	WO 2003-EP9525	20030828
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
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GB 2392910	A	20040317	GB 2003-15870	20030707
CA 2498051	A1	20040325	CA 2003-2498051	20030828

AU 2003282006	A1	20040430	AU 2003-282006	20030828
EP 1546113	A1	20050629	EP 2003-773613	20030828
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JP 2006507355	T	20060302	JP 2004-571738	20030828
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MX 2005PA02644	A	20050920	MX 2005-PA2644	20050309
NO 2005001726	A	20050407	NO 2005-1726	20050407
US 20060160801	A1	20060720	US 2005-527391	20051021
PRIORITY APPLN. INFO.:			GB 2002-20962	A 20020910
			GB 2002-26609	A 20021114
			GB 2003-15870	A 20030707
			WO 2003-EP9525	W 20030828

OTHER SOURCE(S): MARPAT 140:287406  
GI



AB Title compds. I [wherein A = hetero/aryl; R1, R2, R3 = independently H, halo, NO<sub>2</sub>, CN, OH and derivs., (un)substituted alkyl, R4 = CN, trifluoromethylcarbonyl, alkenoxycarbonyl, hydroxycarbonyl, aryl/alkylaminocarbonyl, (un)substituted heteroarylcarbonyl, heterocyclylcarbonyl, heteroaryl, heterocyclyl, alkylcarbonyl, alkoxy carbonyl, mono- and dialkylaminocarbonyl; R5 = NH<sub>2</sub>, (un)substituted alkyl; R6 = H, formyl, N-(alkylsulfonyl)/N-(alkylsulfonyl)-N-(alkyl)/aminocarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, cycloalkylcarbonyl, (un)substituted alkyl, mono- and dialkylaminocarbonyl, alkylcarbonyl, alkoxy carbonyl, heteroaryl, heterocyclyl, etc.; R7 = halo, NO<sub>2</sub>, CN, OH, (un)substituted alkyl, alkoxy; Y1, Y2, Y3, Y4, Y5 = independently CH or N; and their salts, hydrates, and/or solvates, and their tautomeric forms] were prepared as human neutrophil elastase (HNE) inhibitors. For example, II was prepared, in 91% yield, by cyclocondensation of N-[3-(trifluoromethyl)phenyl]urea with 4-cyanobenzaldehyde and Et 3-oxobutanoate. In an in vitro assay, II displayed an IC<sub>50</sub> value of 8 nM for HNE inhibition. Thus, I are useful for treatment of acute and chronic inflammation, ischemic and remodelling processes, in particular chronic obstructive pulmonary diseases.

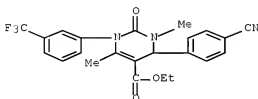
IT 671775-98-7P, Ethyl 4-(4-cyanophenyl)-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate 671776-27-5P 671776-58-2P, 4-(4-Cyanophenyl)-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylic acid

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(human neutrophil elastase inhibitor; preparation of pyrimidinones as human neutrophil elastase inhibitors)

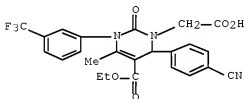
RN 671775-98-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



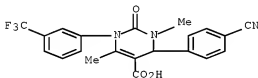
RN 671776-27-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 671776-58-2 ZCAPLUS

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IT 671775-94-3P, Ethyl 4-(4-cyanophenyl)-3-formyl-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate  
 671775-99-8P, Ethyl 3-acetyl-4-(4-cyanophenyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate  
 671776-00-4P, Diethyl 6-(4-cyanophenyl)-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-3,6-dihydro-1,5(2H)-pyrimidinedicarboxylate  
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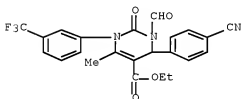
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 671776-81-1P 675103-27-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(human neutrophil elastase inhibitor; preparation of pyrimidinones as human neutrophil elastase inhibitors)

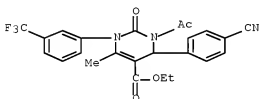
RN 671775-94-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-formyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



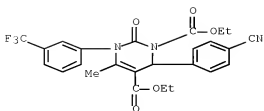
RN 671775-99-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-acetyl-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



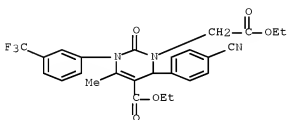
RN 671776-00-4 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,5-diethyl ester (CA INDEX NAME)



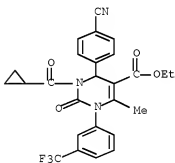
RN 671776-14-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



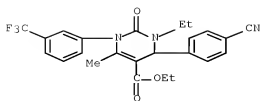
RN 671776-15-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-(cyclopropylcarbonyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



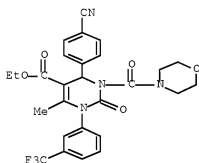
RN 671776-16-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-ethyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



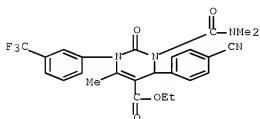
RN 671776-17-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(4-morpholinylcarbonyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 671776-18-4 ZCAPLUS

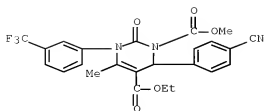
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(dimethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 671776-19-5 ZCAPLUS

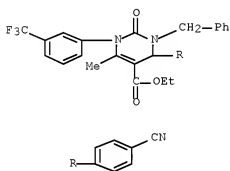
CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-methyl ester (CA INDEX NAME)





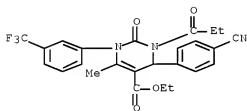
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(phenylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



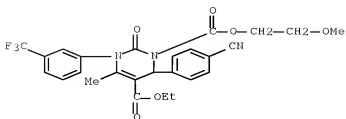
RN 671776-21-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(1-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



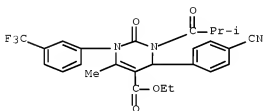
RN 671776-22-0 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-(2-methoxyethyl) ester (CA INDEX NAME)



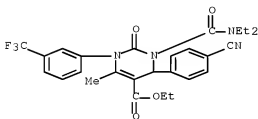
RN 671776-23-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(2-methyl-1-oxopropyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



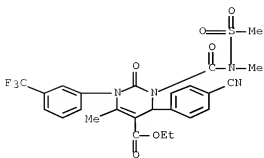
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(diethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



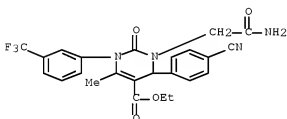
RN 671776-25-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[[methyl(methylsulfonyl)amino]carbonyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



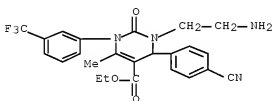
RN 671776-26-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-amino-2-oxoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



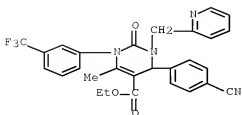
RN 671776-28-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-aminoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



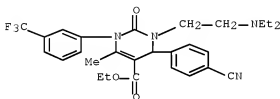
RN 671776-29-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(2-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



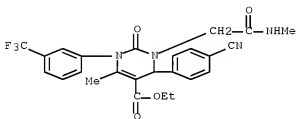
RN 671776-30-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



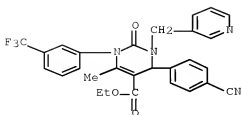
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(methylamino)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



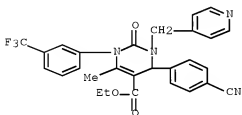
RN 671776-32-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



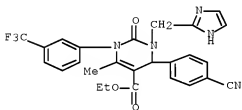
RN 671776-33-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(4-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



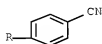
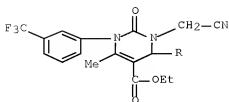
RN 671776-34-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(1H-imidazol-2-ylmethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



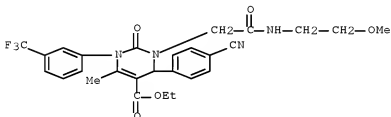
RN 671776-35-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(cyanomethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



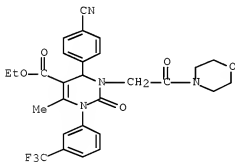
RN 671776-36-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[2-[(2-methoxyethyl)amino]-2-oxoethyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



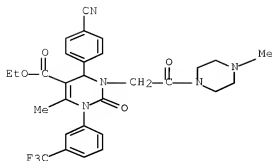
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-morpholinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



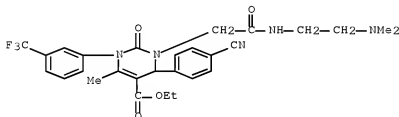
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-methyl-1-piperazinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



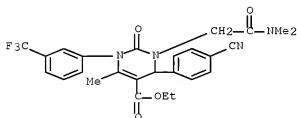
RN 671776-44-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[(2-dimethylamino)ethyl]amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



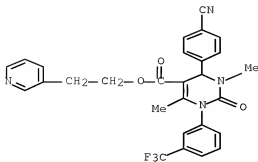
RN 671776-45-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(dimethylamino)-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



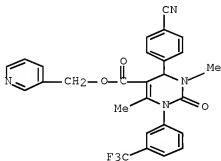
RN 671776-69-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(3-pyridinyl)ethyl ester (CA INDEX NAME)



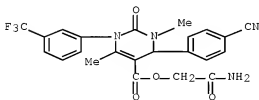
RN 671776-70-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 3-pyridinylmethyl ester (CA INDEX NAME)



RN 671776-71-9 ZCAPLUS

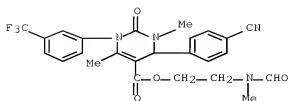
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-amino-2-oxoethyl ester (CA INDEX NAME)



RN 671776-72-0 ZCAPLUS

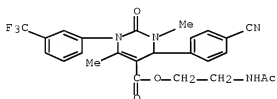
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(formylmethylamino)ethyl ester (CA INDEX NAME)





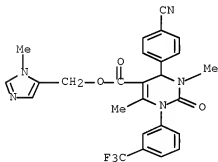
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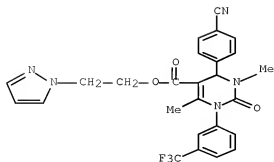
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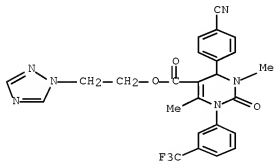
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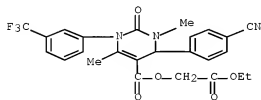
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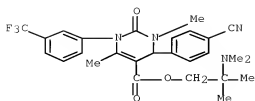
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-ethoxy-2-oxoethyl ester (CA INDEX NAME)



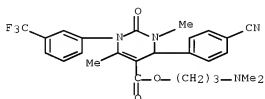
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)-2-methylpropyl ester (CA INDEX NAME)



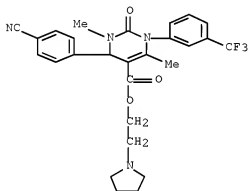
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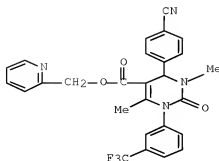
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RN 671776-81-1 ZCAPLUS

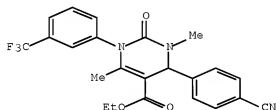
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-pyridinylmethyl ester (CA INDEX NAME)



RN 675103-27-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester, (-)- (CA INDEX NAME)

Rotation (-).



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2004:213317 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 140:253573

TITLE: Preparation of 2-oxypyrimidines as human leukocyte elastase (HNE) inhibitors

INVENTOR(S): Gielen, Heike; Li, Volkhart Min-jian; Rosentreter, Ulrich; Schlemmer, Karl-heinz; Allerheiligen, Swen; Telan, Leila; Baerfacker, Lars; Keldenich, Joerg; Albrecht, Barbara; Meurer, Dirk; Fitzgerald, Mary; Nash, Kevin

PATENT ASSIGNEE(S): Bayer Ag, Germany  
 SOURCE: Brit. UK Pat. Appl., 117 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent  
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

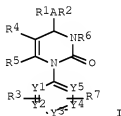
PATENT INFORMATION:

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GB 2392910	A	20040317	GB 2003-15870	20030707
CA 2498051	A1	20040325	CA 2003-2498051	20030828
WO 2004024700	A1	20040325	WO 2003-EP9525	20030828

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 CN 1732159 A 20060208 CN 2003-824983 20030828  
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 PRIORITY APPLN. INFO.: GB 2002-20962 A 20020910  
 GB 2002-26609 A 20021114  
 GB 2003-15870 A 20030707  
 WO 2003-EP9525 W 20030828

OTHER SOURCE(S): MARPAT 140:253573  
 GI



AB Title compds. [I; A = aryl, heteroaryl; R1-R3 = H, OH, halo, NO2, cyano, (substituted) alkyl, alkoxy; R4 = F3CCO, (substituted) alkylcarbonyl, alkoxycarbonyl, alkenyloxy carbonyl, CO2H, arylcarbonyl, heteroaryl, heterocyclyl, cyano, etc.; R5 = (substituted) alkyl, amino; R6 = H, CHO, CONH2, (substituted) alkyl, alkoxy carbonyl, alkylsulfonylaminocarbonyl, heteroaryl, heterocyclyl, etc.; R7 = halo, NO2, cyano, OH, (substituted) alkyl, alkoxy; Y1-Y5 = CH, N, wherein the ring contains 0-2 N], were prepared Thus, 3-trifluoromethylphenylurea, 4-cyanobenzaldehyde, Et 3-oxobutyrate, and polyphosphoric acid Et ester were refluxed 18 h in THF to give 91% Et 4-(4-cyanophenyl)-6-methyl-2-oxo-1-[3- (trifluoromethyl)phenyl]-1,2,3,4-tetrahydro-5-pyrimidinecarboxylate. The latter inhibited HNE with IC50 = 8 nM.

IT 671775-94-2P 671775-98-7P 671775-99-8P  
 671776-00-4P 671776-06-0P 671776-14-0P  
 671776-15-1P 671776-16-2P 671776-17-3P  
 671776-18-4P 671776-19-5P 671776-20-8P  
 671776-21-9P 671776-22-9P 671776-23-1P  
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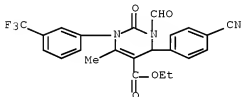
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 671776-75-3P 671776-76-4P 671776-77-5P  
 671776-78-6P 671776-79-7P 671776-80-0P  
 671776-81-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of 2-oxypyrimidines as human leukocyte elastase inhibitors)

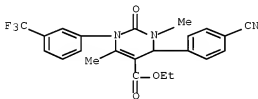
RN 671775-94-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-formyl-1,2,3,4-tetrahydro-  
 6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX  
 NAME)



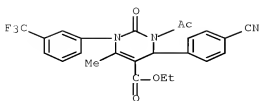
RN 671775-98-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-  
 dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX  
 NAME)



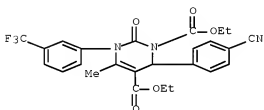
RN 671775-99-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-acetyl-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-  
 6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX  
 NAME)



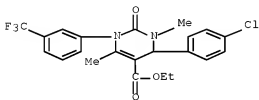
RN 671776-00-4 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 1,5-diethyl ester (CA INDEX NAME)



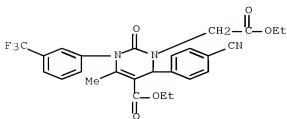
RN 671776-06-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-chlorophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



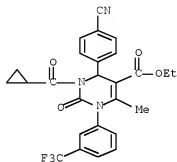
RN 671776-14-0 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



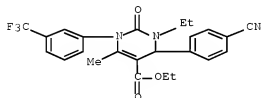
RN 671776-15-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-(cyclopropylcarbonyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



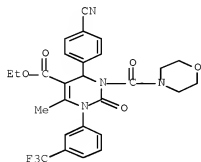
RN 671776-16-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-ethyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 671776-17-3 ZCAPLUS

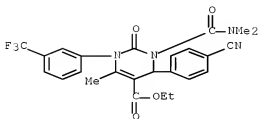
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(4-morpholinylcarbonyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



RN 671776-18-4 ZCAPLUS

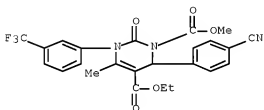


CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(dimethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



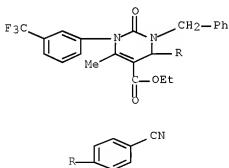
RN 671776-19-5 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-methyl ester (CA INDEX NAME)



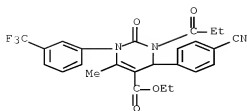
RN 671776-20-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(phenylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



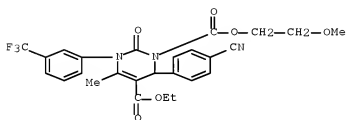
RN 671776-21-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(1-oxopropyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



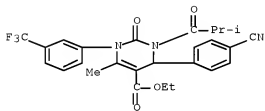
RN 671776-22-0 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 6-(4-cyanophenyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]-, 5-ethyl 1-(2-methoxyethyl) ester (CA INDEX NAME)



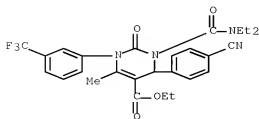
RN 671776-23-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-(2-methyl-1-oxopropyl)-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



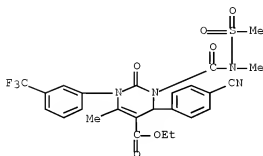
RN 671776-24-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[(diethylamino)carbonyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



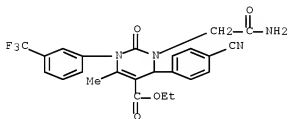
RN 671776-25-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[methyl(methylsulfonyl)amino]carbonyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



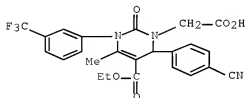
RN 671776-26-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-amino-2-oxoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



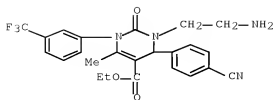
RN 671776-27-5 ZCAPLUS

CN 1(2H)-Pyrimidineacetic acid, 6-(4-cyanophenyl)-5-(ethoxycarbonyl)-3,6-dihydro-4-methyl-2-oxo-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



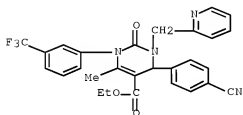
RN 671776-28-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(2-aminoethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



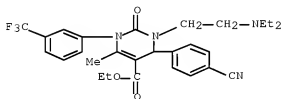
RN 671776-29-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(2-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



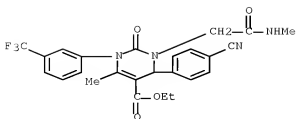
RN 671776-30-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(diethylamino)ethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



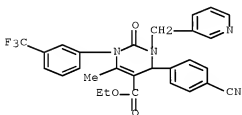
RN 671776-31-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(methylamino)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



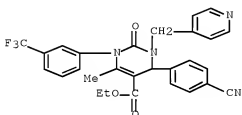
RN 671776-32-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(3-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



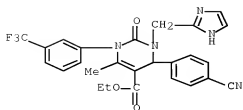
RN 671776-33-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-3-(4-pyridinylmethyl)-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



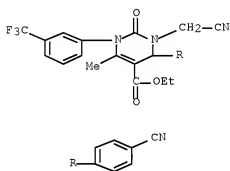
RN 671776-34-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-(1H-imidazol-2-ylmethyl)-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



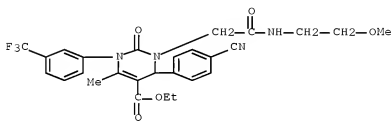
RN 671776-35-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-(cyanomethyl)-4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



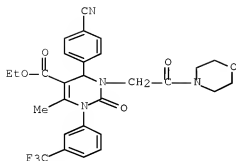
RN 671776-36-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3-[2-[(2-methoxyethyl)amino]-2-oxoethyl]-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



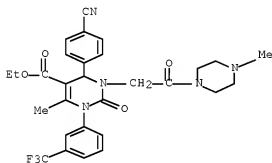
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CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-morpholinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



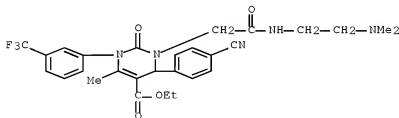
RN 671776-43-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-6-methyl-3-[2-(4-methyl-1-piperazinyl)-2-oxoethyl]-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



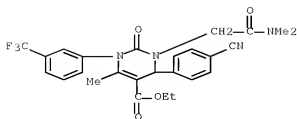
RN 671776-44-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-[(2-(dimethylamino)ethyl)amino]-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



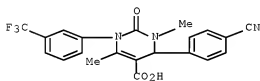
RN 671776-45-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-3-[2-(dimethylamino)-2-oxoethyl]-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, ethyl ester (CA INDEX NAME)



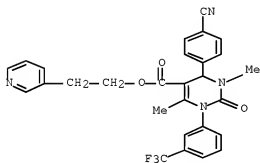
RN 671776-58-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 671776-69-5 ZCAPLUS

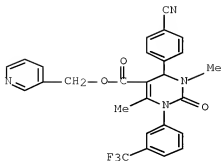
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(3-pyridinyl)ethyl ester (CA INDEX NAME)



RN 671776-70-8 ZCAPLUS

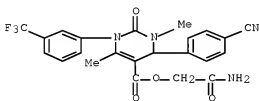
CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 3-pyridinylmethyl ester (CA INDEX NAME)





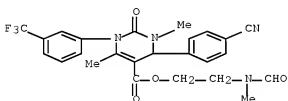
RN 671776-71-9 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-amino-2-oxoethyl ester (CA INDEX NAME)



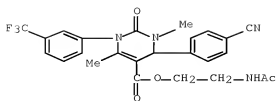
RN 671776-72-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(formylmethylamino)ethyl ester (CA INDEX NAME)



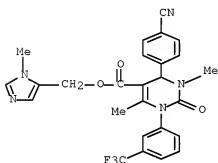
RN 671776-73-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(acetamino)ethyl ester (CA INDEX NAME)



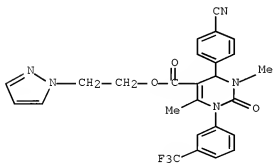
RN 671776-74-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, (1-methyl-1H-imidazol-5-yl)methyl ester (CA INDEX NAME)



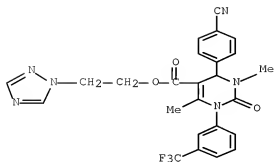
RN 671776-75-3 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1H-pyrazol-1-yl)ethyl ester (CA INDEX NAME)



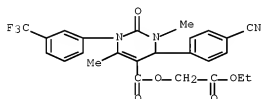
RN 671776-76-4 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1H-1,2,4-triazol-1-yl)ethyl ester (CA INDEX NAME)



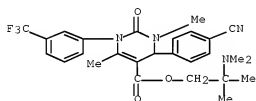
RN 671776-77-5 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-ethoxy-2-oxoethyl ester (CA INDEX NAME)



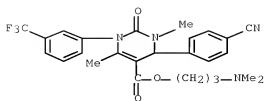
RN 671776-78-6 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(dimethylamino)-2-methylpropyl ester (CA INDEX NAME)



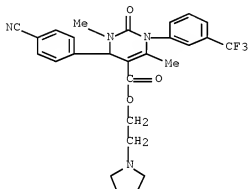
RN 671776-79-7 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 3-(dimethylamino)propyl ester (CA INDEX NAME)



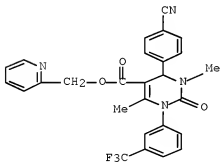
RN 671776-80-0 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-(1-pyrrolidinyl)ethyl ester (CA INDEX NAME)



RN 671776-81-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-1,2,3,4-tetrahydro-3,6-dimethyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-, 2-pyridinylmethyl ester (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

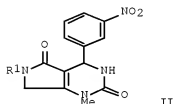
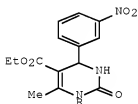
L6 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:779582 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 136:183781

TITLE: Investigation of the chemical reactivity of positions

N-3, C-5 and C-6-methyl group in Biginelli type compounds and synthesis of new dihydropyrimidine derivatives  
 AUTHOR(S): Namazi, H.; Mirzaei, Y. R.; Azamat, H.  
 CORPORATE SOURCE: Lab of Carbohydrates and Biopolymers, Faculty of Chemistry, University of Tabriz, Tabriz, Iran  
 SOURCE: Journal of Heterocyclic Chemistry (2001), 38(5), 1051-1054  
 CODEN: JHTCAD; ISSN: 0022-152X  
 PUBLISHER: HeteroCorporation  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:183781  
 GI

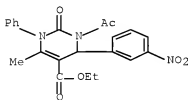


AB Biginelli-type compds. (I; R = Me, Ph) were prepared and converted to eight N-3 substituted dihydropyrimidines using NaH and various electrophiles (ClCO<sub>2</sub>Et, TsCl, Ac<sub>2</sub>O, AcCl and PhCOCl). I (R = Ph) was monobrominated at the C-6-Me group using bromine solution. Reaction of the bromo derivative with amino nucleophiles, such as MeNH<sub>2</sub> and cyclohexylamine, produced two pyrrolopyrimidine derivs. (II; R1 = Me, cyclohexyl). The structures of all the new compds. were confirmed using FTIR, <sup>1</sup>H NMR, and <sup>13</sup>C NMR spectral and elemental analyses.

IT 398456-89-8P 398456-90-1P 398456-91-2P  
 398456-96-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (chemical reactivity of positions N-3, C-5 and C-6-Me group in Biginelli type compds. and synthesis of new dihydropyrimidine derivs.)

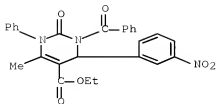
RN 398456-89-8 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-acetyl-1,2,3,4-tetrahydro-6-methyl-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



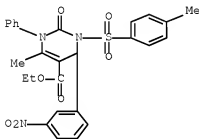
RN 398456-90-1 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 3-benzoyl-1,2,3,4-tetrahydro-6-methyl-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



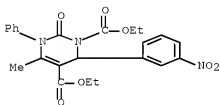
RN 398456-91-2 ZCAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-6-methyl-3-[(4-methylphenyl)sulfonyl]-4-(3-nitrophenyl)-2-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



RN 398456-96-7 ZCAPLUS

CN 1,5(2H)-Pyrimidinedicarboxylic acid, 3,6-dihydro-4-methyl-6-(3-nitrophenyl)-2-oxo-3-phenyl-, 1,5-diethyl ester (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:594082 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:269481

ORIGINAL REFERENCE NO.: 129:54755a,54758a

TITLE: Synthesis and characterization of metal chelates with new pyrimidine derivatives

AUTHOR(S): Siddiqi, K. S.; Nishat, N.

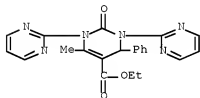
CORPORATE SOURCE: Department of Chemistry, University of Bahrain, Isa Town, Bahrain

SOURCE: Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1998), 28(8), 1353-1369

PUBLISHER: CODEN: SRIMCN; ISSN: 0094-5714  
 DOCUMENT TYPE: Marcel Dekker, Inc.  
 LANGUAGE: Journal  
 English

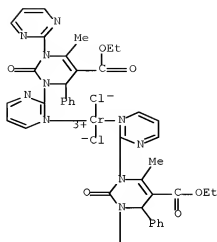
AB The ligands 4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one (L1), 1,3-diacetamido(4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one) (L2) and 1,3-dipyrimidinyl(4-phenyl-5-ethoxycarbonyl-6-methyl-3,4-dihydropyrimidin-2-one) (L3) and their metal chelates with 3d metal ions were synthesized. The conductivity measurements suggest that [M(L1)2Cl2], [M2(L2)Cl4], [M'(L2)Cl6] and [M(L3)2Cl2] are nonelectrolytes in DMSO and MeCN while [M'(L1)2Cl2]Cl and [M'(L3)2Cl2]Cl are 1:1 electrolytes, where M = Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) and M' = Cr(III) and Fe(III). Spectroscopic studies show that L1 coordinates through NH and the O atom of the pyrimidinyl ring, L2 coordinates through the N and O atoms of the amide group while L3 coordinates via the two N atoms of the pyrimidinone ring. The electronic spectra and the magnetic moments reveal that all metal complexes of L1, L3 and complexes of trivalent metal ions with L2 are octahedral while those of the divalent metal ions with L2 probably have a tetrahedral structure except for the Cu(II) complex which appears to be square-planar. The  $\beta$  values suggest a considerable degree of orbital overlap in the metal-ligand bond.

IT 213592-25-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and complexation with first-row transition-metal ions)  
 RN 213592-25-7 ZCAPLUS  
 CN [2,1'(2'H):3'(4'H),2''-Terpyrimidine]-5'-carboxylic acid,  
 4'-methyl-2'-oxo-6'-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



IT 213592-48-4P 213592-50-8P 213592-52-0P  
 213592-54-2P 213592-56-4P 213592-58-6P  
 213592-60-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 213592-48-4 ZCAPLUS  
 CN Chromium(1+), dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-, chloride, (T-4)- (9CI) (CA INDEX NAME)

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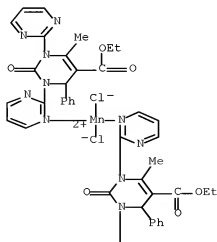


PAGE 2-A



RN 213592-50-8 ZCAPLUS  
 CN Manganese, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-  
 phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-  
 (9CI) (CA INDEX NAME)

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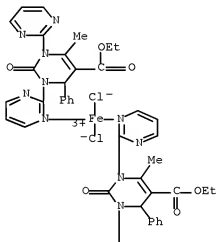
PAGE 2-A



RN 213592-52-0 ZCAPLUS

CN Iron(1+), dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-, chloride (9CI) (CA INDEX NAME)

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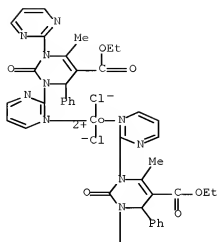
PAGE 2-A



RN 213592-54-2 ZCAPLUS

CN Cobalt, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-, (T-4)- (9CI) (CA INDEX NAME)

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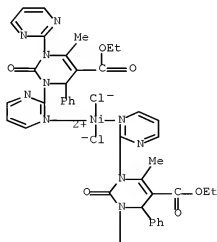
PAGE 2-A



RN 213592-56-4 ZCAPLUS

CN Nickel, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'-(2'H):3'-(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]- (9CI) (CA INDEX NAME)

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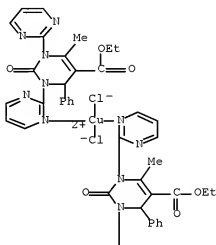
PAGE 2-A



RN 213592-58-6 ZCAPLUS

CN Copper, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]- (9CI) (CA INDEX NAME)

PAGE 1-A



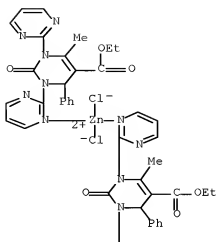
PAGE 2-A



RN 213592-60-0 ZCAPLUS

CN Zinc, dichlorobis[ethyl 6'-methyl-2'-oxo-4'-phenyl[2,1'(2'H):3'(4'H),2''-terpyrimidine]-5'-carboxylate-κN1]-, (T-4)- (9CI) (CA INDEX NAME)

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PAGE 2-A

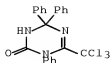


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1976:592595 ZCAPLUS Full-text  
 DOCUMENT NUMBER: 85:192595  
 ORIGINAL REFERENCE NO.: 85:30799a,30802a  
 TITLE: Formation of heterocyclic compounds by use of  
 N'-diphenylmethylene-N-phenyl-N-trimethylsilylurea  
 Matsuda, Isamu; Yamamoto, Sakae; Ishii, Yoshio  
 Fac. Eng., Nagoya Univ., Nagoya, Japan  
 JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANSACTIONS  
 1: ORGANIC AND BIO-ORGANIC CHEMISTRY (1972-1999)  
 (1976), (14), 1523-8  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



II

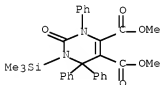


III



IV

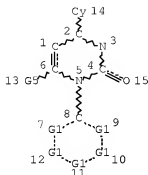
- AB The reactions of the title urea (I) with acceptor mols. were studied. With cyclohexyl isocyanide, MeNCO, MeO2CC.tplbond.CC(=O)Me, or Cl3CCN followed by desilylation I underwent [4+1] or [4+2] cycloaddn.; imidazolidinone, triazinone, and pyrimidinone derivs. were formed. E.g., I with MeNCO gave the triazinone II. I reacted with RCN (R = CC13, NMe2) to give the triazinone III and Ph2C:NC(NMe2):NPh, resp., by decomposition of the intermediate silyloxytriphenyltriazine with MeOH or under the reaction conditions, resp. Reaction of I with RR1CO (RR1 = Ph2C; R = H, R1 = CC13) gave the insertion products Ph2C:NCONPhCRR1OSiMe3. Diketene reacted with I to give the oxazinone IV.
- IT 61032-91-5P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and desilylation of)
- RN 61032-91-5 ZCAPLUS
- CN 4,5-Pyrimidinedicarboxylic acid, 1,2,3,6-tetrahydro-2-oxo-3,6,6-triphenyl-1-(trimethylsilyl)-, dimethyl ester (9CI) (CA INDEX NAME)



FILE 'HOME' ENTERED AT 12:37:08 ON 22 SEP 2008

## SEARCH HISTORY

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L1 STR



VAR G1=C/N  
VAR G5=C/NH2  
NODE ATTRIBUTES:  
CONNECT IS E3 RC AT 1  
CONNECT IS E3 RC AT 3  
DEFAULT MLEVEL IS ATOM  
GGCAT IS UNS AT 14  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE  
L5 397 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 94555 ITERATIONS  
SEARCH TIME: 00.00.04

397 ANSWERS

(FILE 'HOME' ENTERED AT 12:01:55 ON 22 SEP 2008)

FILE 'REGISTRY' ENTERED AT 12:02:08 ON 22 SEP 2008

L1 STR  
L2 8 SEA SSS SAM L1

FILE 'ZCAPLUS' ENTERED AT 12:34:50 ON 22 SEP 2008

L3 3 SEA ABB=ON L2

FILE 'REGISTRY' ENTERED AT 12:34:56 ON 22 SEP 2008

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L6 11 SEA ABB=ON L5

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D STAT QUE L5

FILE 'ZCAPLUS' ENTERED AT 12:36:45 ON 22 SEP 2008  
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D IBIB ABS HITSTR L6 1-11

FILE 'HOME' ENTERED AT 12:37:08 ON 22 SEP 2008  
D STAT QUE L5

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